# **Refreshment Break and Poster Session**

15:30 - 18:00 Monday, 10th June, 2024 Location Tramuntana 1 Presentation type Poster

# **P.001** Synthesis of eco-friendly and biocompatible phospholipid based zwitterionic surfactant possessing antiseptic and antiviral properties from coconut oil source

KiHo Park, JeongMin Lee, <u>JongChoo Lim</u> Dongguk University, Republic of Korea

#### Abstract

The increasing requirement for sustainable technologies due to growing interest for environmental protection and strict environmental control has led to the development of eco-friendly and biocompatible surfactants in various areas including biological and biomedical applications. Increasing concerns over the petroleum resource preservation are also accelerating the development of new eco-friendly and biocompatible surfactants produced from biomass possessing excellent biodegradability, ecological suitability, low toxicity, mildness and high interfacial activity. In this study, an ecofriendly and biocompatible phospholipid based zwitterionic surfactant CDP-W (cocamidopropyl propylene glycol (PG)dimonium chloride phosphate) was synthesized from coconut oil source and the structure of the prepared surfactant CDP-W was identified by FT-IR, 1H-NMR and 13C-NMR analysis. Interfacial property measurements such as critical micelle concentration, static and dynamic surface tensions, interfacial tension, foamability and foam stability have revealed that CDP-W surfactant possesses better surfactant activity and more effective in lowering surface free energy than CAPB (cocamidopropyl betaine) which is a zwitterionic surfactant widely used in cosmetics, personal products and household products. Environmental compatibility tests such as biodegradability, oral toxicity, skin irritation and eye irritation showed that CDP-W surfactant is easily biodegradable, non-toxic, mild and non-irritating to skin and eye. In particular, CDP-W reveals excellent antiseptic and antiviral properties without using any additional preservative and disinfectant, suggesting that CDP-W surfactant can replace CAPB in the formulation of cosmetics, personal products and household products.

## Keywords

Phospholipid based zwitterionic surfactant Coconut oil Antiseptic property Antiviral property

#### Last published paper details

Effect of the Addition of fluorinated surfactant on the solubilization of n-hexane by hydrocarbon surfactant

## Full title of article

Effect of the Addition of fluorinated surfactant on the solubilization of n-hexane by hydrocarbon surfactant

Journal

Applied Chemical Engineering

Year

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#### Volume

34

## First page

397

#### All authors

HeeDong Shin, KiHo Park, JongChoo Lim

## P.002 Molecular aggregation and phase behavior in methane-water mixtures

#### Jiwon Seo, Ravi Singh, Jun-Ho Choi

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#### Abstract

Methane is rarely soluble in water at low pressures, but the solubility is highly increased at very high pressures. For example, the two fluid phases of methane-rich and water-rich exist at 1.3 Gpa, as the pressure further raises into 2.3 Gpa, the two separated fluids change into homogeneous mixture [1]. To explain this unusual methane solubility, methane aggregation behavor was examined in comination study of graph theory and MD simulation [2]. Under lower pressure, methane molecules exhibit a tendecy to form self-associate aggregates while avoiding interaction with water, but formation of spatially extended network is preferred to interact with water at extremely high pressures larger than 2.3 Gpa at 373K. This bifurcating aggregation pathway was already suggested to describe salt solubility [3], water-alcohol miscibility and liquid-liquid phase separation [4] in binary aqueous mixtures. In this work, graph theoretical analysis in various methane-water mixture systems, such as degree distribution, eigenvalue spectrum, is presented to investigate the network properties of methane aggregates and their effect on water structure, and to establish the relationship with methane solubility.

#### REFERENCES

[1] Ciprian G. Pruteanu, Graeme J. Ackland, Wilson C. K. Poon, John S. Loveday, When immiscible becomes miscible-Methane in water at high pressures, Sci. Adv. 3, e1700240, 2017.

[2] Seungeui Choi, Jiwon Seo, Ravi Singh, Jun-Ho Choi, Pressure dependence of molecular aggregation and phase behavior in methane-water mixtures, J. Mol. Liq. 383, 122123, 2023.

[3] Jun-Ho Choi, Hochan Lee, Hyung Ran Choi, and Minhaeng Cho, Graph Theory and Ion and Molecular Aggregations in Aqueous Solutions, Annu. Rev. Phys. Chem. 69, 125, 2018.

[4] Jiwon Seo, Seungeui Choi, Ravi Singh and Jun-Ho Choi, Spatial Inhomogeneity and Molecular Aggregation behavior in Aqueous Binary Liquid Mixtures, J. Mol. Liq. 369, 120949, 2023.

## Keywords

Molecular aggregation Graph theory MD simulation Phase behavior

#### Last published paper details

Pressure dependence of molecular aggregation and phase behavior in methane-water mixtures" Seungeui Choi, Jiwon Seo, Ravi Singh, Jun-Ho Choi, J. Mol. Liq. 383, 122123 (2023)

#### Full title of article

Pressure dependence of molecular aggregation and phase behavior in methane-water mixtures

#### Journal

Journal of Molecular Liquids

#### Year

2023

#### Volume

383

First page

122123

All authors

Seungeui Choi, Jiwon Seo, Ravi Singh, Jun-Ho Choi

# P.003 Polymeric mixed matrix beads with embedded functionalized hydroxyapatite for adsorption of aqueous lead

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## Abstract

The present study showcases a successful synthesis of thiol modified hydroxyapatite (HAp-SH) employing a facile one-step precipitation method. The developed material was characterized in detail using XRD, FTIR, FESEM, EDX and zeta potential analyses. Hap-SH demonstrated increased adsorption capacity for lead (Qmax: 894 mg/g) in water compared to the non-functionalized hydroxyapatite (Qmax: 492 mg/g) which was ascribed to the presence of sulfur groups. The novel powdered adsorbent was further encapsulated in a polyacrylonitrile matrix to develop mixed matrix beads (MMBs) with a Langmuir saturation capacity of 64 mg/g. Additionally, the effect of adsorbent dose, solution pH, temperature along with the adsorption kinetics were elucidated. The adsorption was endothermic in nature and followed pseudo-second order kinetics which indicated a significant role of thiol groups in enhancement of aqueous lead binding capacity. Furthermore, the material showed credible selectivity and reusable properties. Overall, the study emphasizes the promise of the HAp-SH loaded mixed matrix beads for remediation of aqueous lead.

## Keywords

Lead adsorption Functionalized hydroxyapatite Chemisorption

## Last published paper details

UiO-66 is an extremely versatile metal organic framework (MOF) due to its remarkable water stability and high specific surface area. The incorporation of modified chemical and structural defects (missing linker and missing cluster defects) into the crystalline UiO-66 by the simultaneous use of an amino modified ligand and a thiol containing monocarboxylic acid modulator (thioglycolic acid, TGA) during synthesis resulted in developing a novel dual-functional MOF, designated as NH2-UiO-66-SH\_C. This material was characterized using FTIR, XRD, FESEM, EDX, XPS, BET and Zetasizer to explore the morphological integrity and chemical composition. NH2-UiO66-SH\_C crystals demonstrated irregular nano-sized morphology (< 100 nm) and microporous nature with specific surface area of 519.6 m2 /g. The material was subsequently tested to adsorb the highly toxic aqueous mercury (Hg) which is responsible for severe damages to human health. The maximum adsorptive capacity for aqueous inorganic mercury was 885 mg/g at 303 K. The optimum adsorbent dose and solution pH were 0.3 g/L and 5, respectively. The adsorption capacities which were far higher compared to its parent MOFs (UiO-66 as well as NH2-UiO-66) and other reported modified forms of UiO-MOFs. A regeneration method that was effective over 5 cycles (Hg removal efficiency > 90%) was also reported. Overall, this study reports the development of a newly modified nano-crystalline MOF, by manipulation of the synthetic chemistry (with defect modulation), which is a promising adsorbent for Hg (II) in aqueous phase.

## Full title of article

In-situ synthesis of dual functionalized MOF by engineering modulator induced defect for efficient remediation of aqueous mercury through adsorption

#### Journal

#### Year

2023

## Volume

11

## First page

S. Saha Chowdhury, B. Bera, S. De, In-situ synthesis of dual functionalized MOF by engineering modulator induced defect for efficient remediation of aqueous mercury through adsorption, J. Environ. Chem. Eng. 11 (2023) 111332. https://doi.org/10.1016/j.jece.2023.111332.

## All authors

Sayak Saha Chowdhury, Biswajit Bera, Sirshendu De

## DOI

https://doi.org/10.1016/j.jece.2023.111332

# P.004 Hexavalent chromium adsorption in water using amine grafted silica nanoparticles

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## Abstract

Chromium is an extremely toxic carcinogen that disrupts health and environment. The present study addresses the remediation of hexavalent chromium contamination in water with a novel amine (NH<sub>2</sub>) functionalized silicabased adsorbent (designated as PEI-Si). The material was characterized with detailed analyses, such as, FTIR, FESEM, EDS, TGA, BET and zeta potential. PEI-Si demonstrated a high adsorption capacity ( $q_L$ ) of 133.3 mg/g at 25°C and pH 6. The effect of dose, pH and contact time were discussed and the significant contribution of amine groups in the modified adsorbent structure in enhancing the Cr (VI) uptake was shown. The thermal effects and regenerative properties of the adsorbent were also elucidated. Overall, PEI-Si showed credible promise as an efficient adsorbent for treatment of Cr contaminated water.

## Keywords

Grafted silica nanoparticles Amine modification Chromium (VI) capture Chemisorption

## Last published paper details

Explosive detection in aqueous medium using fluorometric titrations is of paramount importance for security and safety, as it offers a susceptible and rapid method to identify potential threats in water sources or aqueous environments, ensuring the protection of critical infrastructure and public safety. Previously, we have investigated fluorescence-based explosive detection via π-electron-rich anthrapyrazolone-derived fluorophore moiety (dye) as an effective sensor in an organic medium. However, the dye's solubility in water makes it difficult to identify nitroaromatics (NACs) in aqueous media. In the current study, thermoresponsive crosslinked polymer (TCP) with dye [DHBBI(MA)2] added as a crosslinker between the polymer chains is synthesised by straightforward and easy free radical polymerization. The emission intensity of TCP is significantly reduced with interaction with NACs like TNP, ATNP, DNP, and PNP, primarily through static quenching attributed to a photoinduced electron transfer (PET) process. TNP exhibited the most efficient quenching, with a Ksv value of 10.7 × 102 M-1 for TCP and 6.189 × 102 M-1 for DHBBI(MA)2. The limit of detection (LOD) was 0.12 nM for TCP and 0.135 nM for DHBBI(MA)2. TCP proved to be approximately 1.72 and 1.12 times more efficient in TNP detection than DHBBI(MA)2 in terms of Ksv value and LOD. At higher temperatures beyond the LCST of the polymer, TCP exhibits additional fluorescence quenching, making it effective for NAC detection. This switch in fluorescence quenching near the cloud point temperature (TCP) of PNIPAM in aqueous media indicates TCP's potential for real-world applications.

Design of smart polymeric sensor based on poly(N-isopropylacrylamide) and anthrapyrazolone derived fluorescent crosslinker for the detection of nitroaromatics in aqueous medium

### Journal

European Polymer Journal

#### Year

2023

### Volume

200

## First page

Design of smart polymeric sensor based on poly(N-isopropylacrylamide) and anthrapyrazolone derived fluorescent crosslinker for the detection of nitroaromatics in aqueous medium, European Polymer Journal, https://doi.org/10.1016/j.eurpolymj.2023.112527. (https://www.sciencedirect.com/science/article/pii/S0014305723007103)

## All authors

Anashwara Babu, Gomathi Sivakumar, Mageshwari Anandan, Prama Adhya, T. Akash, Titash Mondal, Venkatramaiah Nutalapati, Samarendra Maji

## DOI

https://doi.org/10.1016/j.eurpolymj.2023.112527

# **P.005** Scanning probe manipulation and friction measurement of nanodroplets confined by two-dimensional materials

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#### Abstract

Pinning of droplets on solids is an omnipresent phenomenon in nature and in daily life that attracts intense research interest. Understanding the pinning behaviors of droplets is not only academically important but also key for many industrial applications. Here, we investigate the pinning behaviors of nanoscale droplets that are confined by a two-dimensional (2D) elastic sheet onto a substrate by using atomic force microscopy (AFM). The protection provided by the 2D elastic sheet to the droplets makes manipulating them and measuring their pinning forces by a scanning probe possible. This brings the study of the pinning effect of wetting into the micro- and nanometer scales. Our results reveal a time-dependent pinning effect of the confined nanodroplets. The droplets' lateral retention forces are found to increase with increasing their resting times until saturations. Our analysis suggests that dissipation by fine deformations of the substrate, induced by vertical tensions at the contact lines, plays important roles in the droplet's pinning. The creep of the deformation is suggested to result in the time dependence of the droplet's pinning as well as the observed residual ridge structures left by droplets at their original contact lines after their spreads after long resting times.

#### Keywords

Nanoblister Pinning Retection force Atomic force microscopy

#### Last published paper details

Ma, C., Chen, Y., & Chu, J. (2023). Time-dependent pinning of nanoblisters confined by two-dimensional sheets. Part 2: contact line pinning. Langmuir, 39(2), 709-716.

### Full title of article

#### Journal

Langmuir

### Year

2023

### Volume

39

## First page

701

## All authors

C. Ma, Y. Chen, and J. Chu

## P.006 Stability of mustard oil emulsions encapsulated with soy protein and pectin using layerby-layer technique

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## Abstract

Mustard oil has antibacterial, antifungal, and anticancer properties, in addition to health benefits, and is used in the food, pharmaceutical, and cosmetics industries. In the agriculture sector, it can be used as a pesticide. Although mustard oil has several benefits, it can be easily volatilized or oxidized during its use. Oil encapsulation is an alternative to guarantee its effectiveness. In this work, mustard oil was encapsulated using soy protein isolate and high-methoxyl pectin by layer-bylayer technique, and the physical stability, as well as the shelf life of the emulsions, was evaluated. The emulsions were elaborated using protein, pectin, and maltodextrin in pH 3,5. Two oil concentrations were evaluated: 12% (E12) and 37% (E37). Protein was added to the oil and homogenized in Ultra-Turrax at 18.000 rpm for 4 minutes. Next, pectin was added and homogenized under the same conditions to form a bilayer emulsion. The creaming index and droplet size distribution of emulsions were evaluated during 45 days of storage at 25 °C. The emulsions E12 and E37 did not show creaming or physical changes (oil or water separation) after the storage period. Regarding droplet size, E12 had a small increase after 45 days, with diameter increasing from 1.2 to 2 μm. While the E37 had an increase in diameter from 8 μm to 15 μm, in addition to presenting some agglomerates. This increase in droplet size may be associated with coalescence, which results in a subsequent breakdown of the emulsion. In the shelf life study, E12 presented water separation (11.5%) after 180 days of storage, and destabilization after 210 days. The E37 presented unacceptable oil separation after 90 days of storage and destabilization after 120 days. The E12 emulsion was superior to E37, with a very small change in droplet size and remaining stable for a longer period.

## Keywords

Microencapsulation Biopolymers Mustard oil Bilayer emulsion

#### Last published paper details

https://www.sciencedirect.com/science/article/abs/pii/S0268005X19319903#:~:text=Chickpea%20protein%20and%20pecti n%20form%20complexes%20at%20the%20oil%2Fwater%20interface.&text=Increased%20intermolecular%20interactions %20occur%20in%20chickpea%2Dpectin%20interfacial%20films.&text=Chickpea%2Dpectin%20stabilize%20droplet%20si ze,coalescence%20in%20spray%2Ddried%20emulsions.&text=Conjugated%20dienes%20increase%20during%20storage %20of%20microencapsulated%20buriti%20oil.

## Full title of article

Functional properties of chickpea protein-pectin interfacial complex in buriti oil emulsions and spray dried microcapsules

#### Journal

Food Hydrocolloids

#### Year

2020

### Volume

107

## First page

https://www.sciencedirect.com/science/article/abs/pii/S0268005X19319903#:~:text=Chickpea%20protein%20and%20pecti n%20form%20complexes%20at%20the%20oil%2Fwater%20interface.&text=Increased%20intermolecular%20interactions %20occur%20in%20chickpea%2Dpectin%20interfacial%20films.&text=Chickpea%2Dpectin%20stabilize%20droplet%20si ze,coalescence%20in%20spray%2Ddried%20emulsions.&text=Conjugated%20dienes%20increase%20during%20storage %20of%20microencapsulated%20buriti%20oil.

## All authors

Poliana Moser, Vânia Regina Nicoletti, Stephan Drusch, Monika Brückner-Gühmann

## DOI

https://doi.org/10.1016/j.foodhyd.2020.105929

# P.007 Enhancing fullerene content impact on polyurethane resins: Exploring rheological and thermal properties

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## Abstract

Polyurethanes (PUs), rigid or soft, are based on their chemical composition and have a wide range of applications, including building, construction, adhesives, coatings, furniture, and medicine .The coatings based on PUs exhibit high performance and are widely used for concrete, wood, and metals. In this study, the effect of the fullerene content on the properties of different PUs was investigated. Factors affecting the rheological and thermal properties of the prepared polyurethane/ fullerene composites were studied using different kinds of isocyanates and polyols.

The effect of different contents of fullerene on the properties of polyurethane resins (PUs), including rheology and thermal properties, was investigated. The polyurethane resins were prepared through polyaddition reaction using different isocyanate monomers such as isophorone diisocyanate (IPDI), methylene diphenyl diisocyanate (MDI), hexamethylene diisocyanate (HDI), and different polyols such as poly(oxytetramethylene) glycol (PTMG), triol trade name (FA-703), and polypropylene glycols (PPG) at NCO/OH ratio 0.94 and temperature 100 °C. IR spectroscopy was used to control the polymerization reaction of PUs through the shifting of NCO peaks. The results showed that the rheology and thermal properties of the prepared PU resins depend on the type of isocyanates and fullerene used. Based on the type of isocyanates investigated. On the other hand, the PU resin prepared by IPDI and mixed with fullerene has the highest viscosity and thermal stability. However, the initial decomposition temperature (T onset) of the PUs decreased with the addition of fullerene without affecting the maximum decomposition temperature ( $PDT_{max}$ ) of the PU resin.

## Keywords

Polyurethane Fullerene Isocyanate Rheology/Thermal properties

## Last published paper details

### Full title of article

The study of deuterium permeability of film-forming inhibitors with the addition of fullerenes

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International Journal of Hydrogen Energy

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## First page

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## All authors

Nazym Akhanova, Yerassyl Yerlanuly, Didar Batryshev, Timur Kulsartov, Yevgeniy Chikhray, Tlekkabul Ramazanov, Ayfer Veziroglu, Dmitry Schur, Wanli Kang, Maratbek Gabdullin

# DOI

https://doi.org/10.1016/j.ijhydene.2020.11.241

# P.008 Investigating roles of oil pre-oxidation on emulsion stability: Dispersed-phase and interfacial-film both matter

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## Abstract

The inadvertent flow of mildly/moderately oxidized oil into production critically causes quality uncontrollability in food emulsions. In this paper, we explored the effects of oil pre-oxidation (oxidized before emulsification) on the emulsion stability and interfacial properties of two protein emulsifiers (myofibrillar protein, MP; sodium caseinate, SC). These effects were further found to be different dependent on the proteins native structural and physicochemical properties. For MP with a highly structured fibrous conformation, the adsorption capacity, diffusion and rearrangement rate, and dilatational elastic modulus were decreased (by at least 5.74%, 16.25%, 11.21%, 10.04% respectively) at the oxidized-oil/water interface, which were mainly explained by the increased oil polarity and the generated interfacial-active oxidation products that impeded the interfacial unfolding and protein-protein interactions. With an appreciably high adsorbed amount (adsorption ratio > 90%), the MP's oxidized-oil emulsion stability was largely determined by the interfacial properties, and thus significantly decreased with oil oxidation (even at the mild oxidation level). In contrast, for SC with a disordered structure, the rearrangement rate and dilatational elastic modulus were similarly decreased (by at least 14.61%, 12.56% respectively) at the oxidized-oil/water interface, while the adsorption capacity and diffusion rate were increased (by at least 5.40%, 13.16% respectively) possibly due to the enhanced hydrogen bonding between the more hydrophilic SC and the higher polarity oil. With a significantly lower adsorbed amount (adsorption ratio < 10%), the SC's oxidized-oil emulsion stability was mainly decided by the oil inherent properties but not interfacial performance, which thus significantly increased with oil oxidation (even at the mild level) due to the growing oil polarity and density. These findings highlight that mild oil pre-oxidation could have critical impacts on emulsion stability, and the mechanism exploration provides scientific guidelines for the quality control and rational formulation of labile unsaturated oil-based emulsion foods.

## Keywords

Oil oxidation Emulsion stability Adsorption dynamics Interfacial rheology Zhang, W. Y., Zhang, Y. H., He, Y. F., Xu, X. L., & Zhao, X. (2024). Oil density and viscosity affect emulsion stability and destabilization mechanism. Journal of Food Engineering, 366, 111864.

## Full title of article

Oil density and viscosity affect emulsion stability and destabilization mechanism

### Journal

Journal of Food Engineering

### Year

2023

## Volume

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## First page

111864

## All authors

Weiyi Zhang, Yinghao Zhang, Yifei He, Xinglian Xu\*, Xue Zhao\*\*

# DOI

10.1016/j.jfoodeng.2023.111864

# P.010 Hybrid crystalline smart cubosome with nanochannels encapsulating a bioactive from aloe vera

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## Abstract

Smart nanocarrier based bioactive delivery systems are a current focus in nanomedicine for allowing and boosting diverse disease treatments. In this context, designed hybrid lipid-polymer particles can provide structure sensitive features for tailored, triggered and stimuli-responsive devices. Herein, we present a hybrid lipid cubosome surface-modified by complex coacervates of chitosan-*N*-arginine and alginate as a pH-responsive biopolymers shell while acemannan, a bioactive polysaccharide from aloe vera, was encapsulated in the crystalline bioparticle nanochannels with high efficiency and of prolonged release in simulated gastric and intestinal pH conditions. Moreover, crystalline phase transition from Im3m cubic symmetry to inverse hexagonal H<sub>II</sub> promoted by the natural source polysaccharide provides means for

triggering bioactive delivery by further shortening of lattice distances in the cubosome water nanochannels and thus water squeezing out. The bioparticle effective interaction with lipid membrane of high curvature is thermodynamically driven and in the same membrane of low curvature leads to severe morphological changes on giant vesicles as a proof of fusional process yielding tremendous membrane fluidity alteration, hence providing instance for the bioparticles encapsulation in new formed relative smaller vesicles and uptake. Wholly, the structure responsive behavior of a smart bioparticle as an active membrane changer provides applicability perspectives as a triggering delivery device for gastrointestinal tract and further as cell modulator and internalization promoter.

## Keywords

Smart nanoparticle Liquid crystalline phase transition Triggered drug delivery Cell uptake

Last published paper details

Journal of Materials Chemistry B, 2023, 11, 2490-2503

## Full title of article

Interaction of polyelectrolyte-shell cubosomes with serum albumin for triggering drug release in gastrointestinal cancer

## Journal

Journal of Materials Chemistry B

## Year

2023

# Volume

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# First page

2490

# All authors

Barbara Pimenta, Rafael Madrid, Patrick Mathews, Karin Riske, Watson Loh, Borislav Angelov, Angelina Angelova, Omar Mertins

# DOI

10.1039/d2tb02670h

# P.011 Injectable magnesium oxychloride cement foam-derived scaffold for augmenting osteoporotic defect repair

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# Abstract

Cement augmentation has been widely applied to promote osteoporotic fracture healing. whereas the existing calcium-based products suffer from the excessively slow degradation. which may impede bone regeneration. Magnesium oxychloride cement (MOC) has attracted immense attention in tissue-engineering field owing to its promising biological behaviors, but the related study remains limited. Here, a hierarchical porous MOC foam (MOCF)derived scaffold with a more appropriate bio-resorption kinetic and superior bioactivity is presented. Through one-step Pickering foaming, the macro-/micro- two-tier porosity is introduced into the MOC bulk to meet the essential requirement as bone substitute for bone defect repair. The developed MOCF shows excellent handling performance in the paste state, while exhibiting sufficient load-bearing capacity after solidification. In comparison with the traditional bone cement, calcium deficient hydroxyapatite (CDHA), our porous MOCF scaffold demonstrates a much higher biodegradation tendency and better cell recruitment ability. Additionally, the eluted bioactive ions by MOCF commits to a biologically inductive microenvironment, where the in vitro osteogenesis is significantly enhanced. It is anticipated that this advanced MOCF scaffold will be competitive for clinical therapies to augment osteoporotic bone regeneration.



## Keywords

magnesium oxychloride cement foam Pickering foaming technique 3D hierarchical porous scaffold osteoporotic bone repair

## Last published paper details

Yuwei Zhu, Jiaxin Guo, Yifeng Sheng, Jiankun Xu, Ling Qin, and To Ngai. Injectable magnesium oxychloride cement foamderived scaffold for augmenting osteoporotic defect repair. Journal of Colloid and Interface Science. 2023, 640, 199-210. https://doi.org/10.1016/j.jcis.2023.02.109.

## Full title of article

Injectable magnesium oxychloride cement foam-derived scaffold for augmenting osteoporotic defect repair

#### Journal

Journal of Colloid and Interface Science

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#### First page

199

## All authors

Y. Zhu, J. Guo, Y. Sheng, J. Xu, L. Qin\*, T. Ngai\*

## DOI

10.1016/j.jcis.2023.02.109

# P.012 Advanced wearable electronic skin with multifunctional and flexible smart sensors utilizing conjugated polymer nanocomposites

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# Abstract

In the rapidly advancing world of technology, there is a growing global focus on advanced health and environmental monitoring. Wearable and flexible sensors, known for their monitoring abilities, have seen a significant expansion and extensive research in areas like health monitoring, motion detection, and environmental sensing. These sensors require substrates that mimic human skin, characterized by high stretchability, exceptional elasticity, and self-healing features. This research presents the successful development of a self-healing bio-based polyurethane elastomer. This material gains self-healing properties through the incorporation of dynamic disulfide bonds and a hydrogen-bonded cross-linking network. The polyurethane elastomer exhibits superior mechanical strength and elongation capabilities. Furthermore, it demonstrates effective self-repairing ability at room temperature after experiencing cracks. The advanced smart sensor is crafted by embedding conjugated molecules with unique surface textures onto the self-healing polyurethane base, resulting in remarkable pressure sensitivity, mechanical durability, and electrical performance. This multifunctional smart sensor is engineered to detect various stimuli such as strain and pressure, paving the way for revolutionary high-precision health monitoring.

## Keywords

electronic skin flexible sensor bio-based self-healing

#### Last published paper details

Chen, Yen-Chuan, et al. "A crosslinked waterborne poly (vinyl acetate) for greenhouse gas fixation with improved elastomeric properties, shape-memory ability, and recyclability." Journal of Environmental Chemical Engineering 11.6 (2023): 111170.

## Full title of article

A crosslinked waterborne poly(vinyl acetate) for greenhouse gas fixation with improved elastomeric properties, shapememory ability, and recyclability

#### Journal

Journal of Environmental Chemical Engineering

#### Year

2023

#### Volume

11

## First page

111170

## All authors

Yen-Chuan Chen, Ying-Chi Huang, Yi-Hua Huang, Ying-Feng Lin, Ho-Ching Huang, Ru-Jong Jeng, Yu-Wei Cheng, Chien-Hsin Wu

# P.013 Gold nanoparticles functionalized with thiol end-group dendritic polymers on graphene substrates for SERS detection

Kuan-Syun Wang<sup>1</sup>, Ding-Jia Yueh<sup>1</sup>, Ying-Jun Lin<sup>1</sup>, Ting-Yu Liu<sup>1,2,3</sup>

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## Abstract

Novel surface-enhanced Raman scattering (SERS) detection platforms have been fabricated by integrating uniform gold nanoparticle (AuNP) arrays embedded on thiol-terminated dendrons tethered to amino-functionalized graphene. This serves as the basis for SERS system for enhanced analyte detection. Leveraging the modularity of 4-isocyanato-4'-(3,3dimethyl-2,4-dioxo-azetidino)-diphenylmethane (IDD), iterative syntheses yielded bromo-terminated dendrons of varying generations (DG0.5-Br and DG1.5-Br). Subsequent substitution reactions afforded thiol-terminal counterparts (DG0.5-SH and DG1.5-SH). These precisely synthesized 0.5 and 1.5 generation polys(urea/malonamide) dendrons were grafted onto amino-functionalized graphene via ring-opening reactions, followed by AuNP assembly through chemical bonding. The interparticle gaps of AuNPs were precisely tuned by manipulating dendron generation and AuNP size, enabling optimal SERS enhancement. Furthermore, diethylenetriamine (DETA) modification transformed graphene oxide (GO) into aminofunctionalized graphene oxide, facilitating dendron grafting. The controllable interparticle gaps, facilitated by dendron generation and AuNP size, enabled optimal SERS enhancement on thiol-terminated dendrons. Notably, DG0.5-SH exhibited superior AuNP dispersion, leading to exceptional SERS performance. Additionally, laser-induced graphene (LIG) proved more effective than thin-film graphene in SERS enhancement due to its 3D structure and efficient signal reflection. The LIG-based SERS substrate, with its 3D porous architecture, enables rapid and stable SERS detection of liquid analytes, demonstrating significant potential for biomolecule and environmental pollutant analysis in real-world applications.

## Keywords

Surface-enhanced Raman scattering (SERS) detection Thiol-end group dendrons Gold nanoparticle precise synthesis

#### Last published paper details

Wang, K. S., Kuan, T. Y., Chen, Y. C., Chu, Y. J., Chen, J. S., Chen, C. C., & Liu, T. Y. (2024). Simultaneous detection of SARS-CoV-2 S1 protein by using flexible electrochemical and Raman enhancing biochip. Biosensors and Bioelectronics, 116021.

#### Full title of article

Simultaneous detection of SARS-CoV-2 S1 protein by using flexible electrochemical and Raman enhancing biochip

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# **P.014** Preparation of a plastic surface displaying amino groups and reuse of the surface through degradation

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## Abstract

A plastic surface displaying amino groups is valuable because it can be used as a biosensor and a catalytic surface. However, once used, a substrate must be disposed of. In this study, we attempted to develop a reusable plastic surface displaying amino groups. We introduced a degradable copolymer with amino groups onto a plastic surface using the dipcoating method. We examined the reusability of the functionalized surface through the surface degradation.

We synthesized  $poly(CL-r-(Boc)OC-C_6N)$ , a copolymer with ester bonds in the main chain backbone and amino groups protected by Boc groups in the side chain. A  $poly(CL-r-(Boc)OC-C_6N)$  -coating film was prepared on a PET substrate by the dip-coating method. The amino groups displayed on a surface of a PET substrate were prepared by deprotecting the Boc groups. To modify the substrate surface with perfluoroalkyl groups, a fluorinating compound, Rf8-COCI, which had a perfluoroalkyl group, was reacted with amino groups on the surface. XPS measurements observed a fluorine peak (F1s) on the modified surface, indicating that the fluorine modification was successfully achieved.

The reusability of the surface of the PET substrate displaying amino groups was investigated using the fluorine-modified surface. The surface was degraded using 1 M NaOH aq. to remove the fluorine-modified surface layer. In the XPS measurements, the F1s peak observed on the fluorine-modified surface disappeared after the degradation. The substrate surface after the degradation was modified again with Rf8-COCI. The F1s peak was again observed on the surface of the re-fluorinated substrate by XPS measurements. The results demonstrated the surface of the PET substrate displaying amino groups was again modified with perfluoroalkyl groups. These above results indicated that the surface of the PET substrate displaying amino groups was renewed through the degradation of the coated polymers and reused for the surface functionalization.

## Keywords

Amino groups Surface Degradable polymer Reusable

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# **P.015** D-peptide that forms a stereocomplex with amyloid $\beta$ inhibits the fibril formation

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## Abstract

Alzheimer's disease (AD) is the most common form of dementia worldwide. Conventional medicines for AD can only "delay" the progression of dementia to a small extent. Hence, therapeutics that can fully cure AD is required as our society keeps aging. However, the development of a medicine for AD has been difficult, since the mechanism of AD is still unclear. The amyloid cascade is the most supported hypothesis for the onset of AD, in which amyloid  $\beta$  (A $\beta$ ) monomers aggregate to form A $\beta$ -oligomers, ultimately resulting in insoluble A $\beta$ -fibrils. These A $\beta$  aggregates are toxic, and are thought to be responsible for neuronal cell death, leading to dementia. We thought that the inhibition of the aggregation of A $\beta$  molecules would prevent the progression of AD. In this study, we attempted to inhibit A $\beta$  aggregation using peptides consisted of D-amino acid residues (D-peptides) by forming a stereocomplex between A $\beta$  and the D-peptides. A stereocomplex is a complex formed by a stereoselective interaction between two complementing stereoregular polymers. Our group recently found that short L- and D-peptides could also form a stereocomplex with hydrophobic and electrostatic interactions enhanced by stereochemistry. We here synthesized D-peptides consisted of D-phenylalanine and D-arginine with the N-termini acetylated and C-termini amidated. The D-peptides were designed to interact with A $\beta$  to form stereocomplexes and to give electrostatic repulsion between the complexes. We evaluated the effects of the designed D-peptides on the inhibition of A $\beta$  aggregation.

## Keywords

Amyloid β D-peptide Alzheimer's disease

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# P.016 Quantification and control of the surface density of a clickable azide group presented by functional polymer coating

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## Abstract

Strain-promoted azide-alkyne cycloaddition (SPAAC) is a type of Huisgen 1,3-dipolar cycloaddition reaction, also known as a copper-free click reaction. SPAAC is widely used for the modification of biomolecules such as proteins, DNA and cells. It is a bioorthogonal reaction that does not affect various functional groups in living organisms and it does not use cytotoxic copper catalysts. In our previous study, cyclic alkyne groups were presented on a plastic substrate by coating a functional polymer, and DNA molecules were successfully immobilized via SPAAC<sup>[1]</sup>. In this study, azide groups were presented on a surface of a plastic substrate by coating a functional polymer. Then, we quantified the density of azide groups presented on the substrate surface using cyclic alkyne-modified fluorescein, and controlled the surface density of azide groups by blending polymers for coating. In addition, a surface patterned with azide groups was prepared on a substrate surface by microcontact printing ( $\mu$ CP).

## Keywords

Surface Coating Click chemistry Patterning

## Last published paper details

Morita, K. et al. Cellulose 30, 11357-11367 (2023).

## Full title of article

Nanoscopic lignin mapping on cellulose nanofibers via scanning transmission electron microscopy and atomic force microscopy

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## All authors

K. Morita, M. Takenaka, K. Tomita, J. Ishii, H. Kawaguchi, D. Murakami, H. Amo, M. Fujii, T. Maruyama, T. Matsumoto, T. Nishino, and C. Ogino

# DOI

# P.017 Induction of apoptosis in cancer cells by self-assembled forms of small molecule compounds

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## Abstract

Today, chemotherapy using anti-cancer drugs is commonly used as a treatment for cancer. However, anti-cancer drugs also affect normal cells, causing side effects that are problematic. In this study, we focused on apoptosis, which is one of mechanisms of cell death, and attempted to develop a new molecule that induces cell apoptosis. A previous study reported by another group demonstrated that a molecule called 1541B self-assembled to form nanofibers and that procaspase-3 was adsorbed on the nanofibers and activated to produce caspase-3<sup>[1]</sup>. The activation of caspase-3 is closely related to apoptosis. The objective of this study was to develop novel self-assembling molecules with a simpler chemical structure inspired by 1541B. We synthesized a series of compounds that had a part of the molecular structure of 1541B and evaluated their induction of apoptosis in cancer cells.

To explore the apoptosis pathway, we used various caspase substrates to detect caspase activation in HepG2 cells (human liver cancer cells). The results showed that IPP- $C_{14}$  induced caspase-3 activation in HepG2 cells. However, no activation of purified procaspase-3 (without living cells) was observed using IPP- $C_{14}$ . These suggested that, in contrast to the previous study, IPP- $C_{14}$  was not directly related to the activation of caspase-3 in the cells. Then, we looked at the activation of caspase-10, which is upstream of caspase-3. Activation assays using the caspase-10 substrate suggested that IPP- $C_{14}$  induced the activation of caspase-10 in HepG2 cells. These results suggest that IPP- $C_{14}$  indirectly induced the activation of caspase-3 by activating caspase-10 in HepG2 cells, finally leading to their apoptosis.

Other investigations indicated that the molecular aggregation of IPP- $C_{14}$  was essential for the induction of apoptosis. In the poster presentation, we will provide the detail insight on the apoptosis induced by IPP- $C_{14}$ .

[1] Zorn et al., J. Am. Chem. Soc, 133, 19630 (2011)

## Keywords

Apoptosis Caspase Self-assembly Fas receptor

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# P.018 Development, optimization and stabilization of BTK-inhibitor loaded PEGylated colloidal vesicles: Application of quality by design and lyophilization

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## Abstract

Inhibition of Bruton's tyrosine kinase (BTK) plays a vital role in restoring T cell-dependent anti-tumor immune response against various types of cancers. However, the potential of the current treatment is obscured due to its off-target toxicity and low oral bioavailability. Liposomes, the well-known colloidal vesicles, thus become a suitable choice of drug delivery as they have proven their clinical prowess through the parenteral route. However, aqueous liposomes possess limited physicochemical stability and undergo rapid elimination from systemic circulation. Therefore, the preparation of drugloaded liposomes with specific quality attributes and required stability is of utmost importance for desirable clinical outcomes. Thus, to overcome these issues and develop liposomes for better translational aspects, we developed lyophilized BTK-inhibitor-loaded PEGylated liposomes. For this, critical formulation and process parameters were optimized using QbD/DoE techniques. The developed aqueous colloidal formulation was then subjected to a meticulously developed lyophilization process to obtain a stable liposomal drug product. Lyophilization recipe was designed based on selecting a suitable cryoprotectant and the critical glass transition temperature of the liposomal dispersion. The optimized lyophilized liposomal formulation was further characterized to evaluate its physicochemical attributes. The developed formulation exhibited %entrapment efficiency and particle size of 87.33% and 210 nm, respectively, suiting the targeted product profile. The optimized PEGylated liposomes demonstrated a PEG-layer thickness of 2.82 nm. Stability studies of the developed formulation were conducted for a period of 6-months at various storage conditions. The aqueous colloidal dispersion exhibited a significant %degradation of 16-36% at 25°C/60%RH, which was reduced to less than 1% in lyophilized formulation. Thus, investigating the behavior of PEGylated liposomes upon lyophilization from the stability perspective helped us gain insights into the dynamic nature of this spontaneous colloidal system. The developed lyophilized liposomal formulation showcased enhanced stability and retention of its physicochemical attributes, implying its translational possibilities.

## Keywords

Colloidal dispersion Lyophilization Liposomes QbD

#### Last published paper details

S Rani, RK Sahoo, A Mahale, K Panchal, A Chaurasiya, O Kulkarni, K Kuche, S Jain, KT Nakhate, Ajazuddin, Gupta U. (2023). Sialic Acid Engineered Prodrug Nanoparticles for Codelivery of Bortezomib and Selenium in Tumor Bearing Mice. Bioconjugate chemistry, 34(9), 1528–1552. https://doi.org/10.1021/acs.bioconjchem.3c00210

## Full title of article

Sialic Acid Engineered Prodrug Nanoparticles for Codelivery of Bortezomib and Selenium in Tumor Bearing Mice

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## All authors

Sarita Rani, Rakesh K Sahoo, Ashutosh Mahale, Kanan Panchal, Akash Chaurasiya, Onkar Kulkarni, Kaushik Kuche, Sanyog Jain, Kartik T Nakhate, Ajazuddin, Umesh Gupta

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# P.019 Cell-interlinked 3D macroporous annealed particle scaffolds based on porous dextran microgels

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## Abstract

Creating functional human tissue models for drug discovery and regenerative medicine involves replicating native tissue structure using a combination of various cell types and 3D scaffolds. Hydrogels have emerged as a versatile platform for this purpose, offering customizable mechanical properties and essential biochemical cues that promote cell adhesion and growth. Traditionally, nanoporous hydrogels have been employed, but they come with limitations. To address these limitations, macroporous annealed particle scaffolds (MAP) have been developed. This technique involves assembling micron-sized colloidal hydrogels (microgels), and chemically interlinking them to create macroporous structures with interconnected pores. The resulting interstitial spaces are critical for enabling effective cell-cell interactions. However, existing MAP scaffolds come with limitations. The depth of cell infiltration and the available space for cell growth within these scaffolds are predetermined during assembly, which hinders uniform cell distribution and cell-cell interactions. Furthermore, the lack of porosity of most synthetic hydrogels does not allow for sufficient nutrient support towards the center of MAP assemblies. In this study, we introduce a novel cell-induced interlinking method of dextran microgels to generate MAP scaffolds. This innovative approach eliminates the need for chemical crosslinkers and pre-engineered pores to create micro- or macropores within these 3D frameworks. It offers several advantages over previous techniques, allowing cells to self-organize alongside microgels to form dynamic tissue constructs. Moreover, the tunable porosity of the microgels obtained through microfluidic techniques provide higher diffusion of nutrients inside the MAP scaffold. Our study demonstrates the versatility of our approach by showcasing the ability to control scaffold shape and volume by adjusting the cell/microgel ratio and microgel stiffness. In conclusion, our study presents an innovative approach to 3D MAP scaffold development, emphasizing cellular self-organization by utilizing bio-based, porous dextran microgels to facilitate uniform cell infiltration and eliminate the need for artificial constraint networks.

## Keywords

biomaterials scaffolds microfluidics 3D cell culture

### Last published paper details

S. Bulut, D. Günther, M. Bund, C. Haats, T. Bissing, C. Bastard, M. Wessling, L. De Laporte, A. Pich, Cellular Architects at Work: Cells Building their Own Microgel Houses. Adv. Healthcare Mater. 2023, 2302957.

#### Full title of article

Cellular Architects at Work: Cells Building their Own Microgel Houses.

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Selin Bulut, Daniel Günther, Michelle Bund, Christina Haats, Thomas Bissing, Céline Bastard, Matthias Wessling, Laura De Laporte, Andrij Pich

# DOI

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# **P.020** A holistic investigation of the consolidation of calcium carbonate using hydrolysed polyacrylamide

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# Abstract

In young carbonate reservoirs, additional consolidation is often required to maintain the reservoirs' structural integrity. This paper discusses a comprehensive experimental study on the consolidation of calcium carbonate (CaCO<sub>3</sub>) via hydrolysed polyacrylamide (HPAM), specifically the F3330 polymer. The research is divided into three main sections. In the first section, the consolidation ability of F3330 on CaCO<sub>3</sub> is investigated under room conditions. Three different systems are studied: a dilute colloidal system (1:25 mass ratio of CaCO<sub>3</sub> to HPAM), a concentrated colloidal system (1:2 mass ratio), and an incubation of Iceland spar calcite crystal in dilute HPAM solution. UV-Vis adsorption, zeta potential, oscillatory rheology in the form of storage modulus (G') and atomic force microscopy (AFM) force mapping, reveal positive interactions and increased consolidation with higher F3330 dosage, up to an optimum level. The second section explores the impact of reservoir conditions, namely salinity and temperature, on F3330's consolidating ability. Similar experiments were conducted as in section one. Salinity tests indicate a higher polymer dosage requirement under increased salt concentration to maintain optimum CaCO<sub>3</sub> consolidation, while temperature tests show a reduction in peak mechanical strength of consolidated CaCO<sub>3</sub> samples due to thermal degradation of F3330. In the third section, the preservation of F3330's applicability in reservoir conditions by crosslinking it with silica nanoparticles (SiONP) was explored. The results from oscillatory rheology demonstrate that CaCO<sub>3</sub> consolidated by crosslinked F3330 retains peak mechanical strength even when treated with brine and subjected to continuous heating for three days. This extensive investigation into the consolidation of CaCO<sub>3</sub> by HPAM, particularly F3330, provides valuable insights into the potential of HPAM for strengthening reservoir rocks, with the novel approach of crosslinking showing promise for preserving HPAM's usability in challenging reservoir conditions.

# Keywords

polyacrylamide calcium carbonate consolidation crosslinking

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Lew, J.H.; Luckham, P.F.; Matar, O.K.; Müller, E.A.; Santos, A.S.; Maung Maung, M.T. Consolidation of Calcium Carbonate Using Polyacrylamides with Different Chemistries. Powders 2024, 3, 1-16. https://doi.org/10.3390/powders3010001

### Full title of article

Consolidation of Calcium Carbonate Using Polyacrylamides with Different Chemistries

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Lew, J.H.; Luckham, P.F.; Matar, O.K.; Müller, E.A.; Santos, A.S.; Maung Maung, M.T.

## DOI

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# P.021 Probing aging and aggregation behaviors of soft colloids at interfaces by evanescent light scattering

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<sup>1</sup>Jiangnan University School of Chemical and Material Engineering Key Laboratory of Synthetic and Biological Colloids, Ministry of Education, China. <sup>2</sup>The Chinese University of Hong Kong Department of Chemistry, Hong Kong

# Abstract

Here, we employed series of speckle images to explore the aggregation behavior, structural relaxation and physical aging of colloids at interfaces or near a surface. These speckle images are created by the scattering lights either from an evanescent field (*i.e.*, the total internal reflection microscopy) or from the bulk directly. A density-fluctuation autocorrelation function was utilized to deduce the characteristic relaxation time. Both stretched and compressed relaxation behaviors are observed under corresponding surface activities. Also, we find the speed of physical aging is highly correlated with the inter-particle interaction, ionic strength, surface wettability and atmospheric conditions like temperature. We first examined the effect of the interfacial wettability on the structural relaxation of one representative soft colloidal system, poly(Nisopropylacrylamide) (PNIPAM) microgels, during colloidal gel evolution within a large range of particle volume fraction  $\phi$ . Relative to the single relaxation in bulk, a two-step relaxation behavior with fast mode and slow mode is observed at hydrophilic and hydrophobic interfaces. Also, the relaxation time obeys distinct power-law dependences on the intermediate regime of scattering vector. Besides, we examined the near-surface aggregation behavior of hard colloids (polystyrene nanoparticles, PSNPs) with soft protein (fibrinogen) corona. Again, the two-step relaxation phenomena emerge. The fast decay may attribute to the interaction between the unstable soft corona and PSNPs, while the slow decay reflects the entire structural relaxation after the

formation of clusters or colloidal networks. Our findings indicate the protein corona strongly affects the stability and aggregation behavior of nanoparticles at interfaces or near a surface.

# Keywords

microgels soft colloids aggregates evanescent light scattering

## Last published paper details

Liu Wei, Zhu Yuwei, Li Yinan, Han Jie, Ngai To (2023). Unveiling the structural relaxation of microgel suspensions at hydrophilic and hydrophobic interfaces. Journal of Colloid and Interface Science, 633, 948-958.

## Full title of article

Unveiling the structural relaxation of microgel suspensions at hydrophilic and hydrophobic interfaces

## Journal

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# All authors

Liu Wei, Zhu Yuwei, Li Yinan, Han Jie, Ngai To

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# P.022 Optimality of poly vinyl alcohol-starch-malic acid blended composite films for wound dressing application

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# Abstract

The optimality of ternary formulations with variant concentrations of starch (St, 4.5 - 10.5 w/w%), polyvinyl alcohol (PVA, 4.5 - 10.5 w/w%), and malic acid (MA, 12 - 43 wt%)] along with a fixed choice of glycerol (18.38 wt%) was targeted to obtain a wound dressing applicable polymeric composite film. The experimental formulations were designed based on central composite design using response surface methodology. The investigation is associated with acquiring proper combinations of the absorbency of the wound exudates, in-vitro degradation of the papered polymeric composite under a hydrolytic environment,

RSM optimized compositions were measured to ensure the applicability of the PVA-St-MA film. The optimized composition refers to high water absorption (583.83 %) and elongation (99.53 %), in-vitro degradation (65.47 %), and mechanical strength (5.57 MPa), along with good prolific activity against HEK cells (181.95 %).

## Keywords

Film composite In-vitro hydrolytic degradation Antibacterial effectiveness In-vitro biocompatibility

## Last published paper details

Das A, Bhattacharyya S, Uppaluri R, Das C (2020) Optimality of poly-vinyl alcohol/starch/glycerol/citric acid in wound dressing applicable composite films. Int J Biol Macromol 155:260–272. https://doi.org/10.1016/j.ijbiomac.2020.03.185

## Full title of article

Optimality of poly-vinyl alcohol/starch/glycerol/citric acid in wound dressing applicable composite films

## Journal

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All authors

A Das , S Bhattacharyya, R Uppaluri , C Das

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https://doi.org/10.1016/j.ijbiomac.2020.03.185

# P.024 Synthesis, characterization and evaluation of chitosan/graphene oxide/curcumin@metal oxides as adsorbents for the removal of Cr(VI) and As(III) from colloidal wastewaters

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## Abstract

Heavy metals are thought to be among the leading harmful mineral contaminants in water. Their contamination became more severe as a result of fast worldwide population increase, and accelerated industrialization, with heavy metal levels in several water media surpassing regulatory guidelines. Among heavy metals, the presence of arsenic (III) produces health problems such as bone marrow, and encephalopathy, while Cr (VI) harms the environment and has catastrophic consequences for human health. Adsorption is a frequently employed approach for removing heavy metals in aquatic environments, because it is renewable, inexpensive and produces no secondary pollution.

Carbon-based nanomaterials have been investigated as superior adsorbents. The current study recommends the usage of adsorbents based on graphene oxide (GO). GO is a one-atom-thick graphitic layer with extraordinary physical, chemical and mechanical characteristics, including a large surface area, thermal and chemical stability. The structural modification of graphene oxide renders it a better candidate for the adsorption process. Metal oxides have a unique affinity for arsenic and chromium. Chitosan's framework contains cationic and anionic functional units, making it innocuous, versatile and easy to modify. Curcumin has been employed as a reduction and conjugating agent for metal oxide nanoparticles.

Their adsorptive efficiency towards As and Cr was evaluated by batch adsorption experiments. The composites' morphology and structure were characterized by FT-IR, SEM, BET and XRD. The effect of solution pH, contact time, temperature and initial concentration on the adsorption of the composites were determined. Two kinetic models were examined to fit the kinetics pseudo first and pseudo second order models and the optimal pH was found. The equilibrium adsorption data at different temperatures were fitted to the Langmuir and Freundlich isotherm models. The results indicate that the composites can be effectively employed for the removal of heavy metals from water.

## Keywords

Graphene oxide Heavy metals Adsorption Wastewaters

## Last published paper details

Y. Dago-Serry, K.N. Maroulas, A.K. Tolkou, N. AbdelAll, A.N. Alodhayb, G.A. Khouqeer\*, G.Z. Kyzas\*, "Composite superadsorbents of chitosan/activated carbon for the removal of nonsteroidal anti-inflammatory drug from wastewaters", Journal of Molecular Structure 1298 (2024) Article number 137044 (doi: 10.1016/j.molstruc.2023.137044)

## Full title of article

Super-hydrophobic chitosan/graphene-based aerogels for oil absorption

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## All authors

K.N. Maroulas, D.G. Trikkaliotis, Z. Metaxa, N. AbdelAll, A.N. Alodhayb, G.A. Khouqeer, G.Z. Kyzas

## DOI

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# **P.025** Cyclic-polymer grafted colloids in spherical confinement: Insights for interphase chromosome organization

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## Abstract

chromosome structures as colloidal particles whose surfaces are grafted by cyclic polymers. The cyclic polymers, with varying polymerization degrees, mimic chromatin loops present in interphase chromosomes, while the rigid core models the chromocenter section of the chromosome. Our simulations show that the colloidal chromosome model provides a well-separated particle distribution without specific attraction between the chain monomers. As the polymerization degree of the grafted cyclic chains decreases while maintaining the total chromosomal length (e.g. the more potent activity of condensinfamily proteins), the average chromosomal volume becomes smaller, inter-chromosomal contacts decrease, and chromocenters organize in a quasi-crystalline order reminiscent of a glassy state. This order weakens for polymer chains with a characteristic size on the order of the confinement radius. Notably, linear-polymer grafted particles also provide the same chromocenter organization scheme. However, unlike linear chains, cyclic chains result in less contact between the polymer layers of neighboring chromosome particles, demonstrating the effect of DNA breaks in altering genome-wide contacts. Our simulations show that polymer-grafted colloidal systems could help decipher 3D genome architecture along with the fractal globular and loop-extrusion models.

## Keywords

molecular dynamics simulations polymer physics chromosome organization

## Last published paper details

Jarosław Paturej and Aykut Erbaş 2023 Phys. Biol. 20 056004

#### Full title of article

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## All authors

J. Paturej and A. Erbas

# P.026 Interfacial phenomena at the interface of Hap/Fe2O3 composite and electrolyte solution

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## Abstract

Phase boundaries are an area where significant changes occur in the structure and properties of materials. Interfacial phenomena at phase boundaries play a key role in the behavior of substances, affecting their chemical reactions, mechanical strength, thermal conductivity and many other properties. Phase boundaries occur where different phases of matter, such as solid, liquid, and gas, meet.

The Hap/Fe<sub>2</sub>O<sub>3</sub> composite is a material that has remarkable adsorption properties. These have already been confirmed for many ions. New to the research, on the other hand, is the adsorption of silver. This element is characterized by a number of properties, including bactericidal activity. This makes it possible to obtain a material with outstanding properties.

What's more, its adsorption capabilities also allow it to be used as a water and wastewater treatment agent. Such aspects are extremely important in today's research.

In this research, we will focus on the analysis of a variety of interfacial phenomena occurring at phase boundaries using methods, i.e. SEM, porosimetry, potentiometric titration, zeta potential measurements, paying attention to their impact on the properties and behavior of materials. Learning about these processes is fundamental not only for understanding basic aspects of physics and chemistry, but also for developing new technologies, improving the quality of materials and designing modern devices and structures.

## Keywords

adsorption composite hydroxyapatite silver

#### Last published paper details

6. A. Biedrzycka, A. Gładysz-Płaska, E. Skwarek. Study of the effect of uranium recovery on the Hap/Fe2O3 composite and the Fe2O3 interface on the parameters of the electrical double layer" J. Mater. Chem. A, 2023; doi: 10.1039/d3ta03890d.

#### Full title of article

Study of the effect of uranium recovery at Hap/Fe2O3 composite and Fe2O3 interfaces on the parameters of the electrical double layer

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Journal of Materials Chemistry A

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#### Volume

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## All authors

Adrianna Biedrzycka, Agnieszka Gładysz-Płaska, Ewa Skwarek

# **P.027** A heterogeneous ZnO structure with Co3O4 as a co-catalyst to improve photoelectrochemical efficiency.

#### Aiymkul Markhabayeva

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## Abstract

Recently, heterostructured photocatalysts have gained significant attention in the field of photo-catalysis due to their superior properties compared to single photocatalysts. One of the key ad-vantages of heterostructured photocatalysts is their ability to enhance charge separation and broaden the absorption spectrum, thereby improving photocatalytic efficiency. Zinc oxide is a widely used n –type semiconductor with a proper photoelectrochemical activity. In this study, zinc oxide nanorod arrays were synthesized, and then the surface of ZnO nanorods was modified with p-type semiconductor  $Co_3O_4$  to create p-n junction heterostructure. A significant increase in the photocurrent for the ZnO/Co<sub>3</sub>O<sub>4</sub> composite by 4.3 times was found compared to pure ZnO. The dependence of photocurrent on the morphology of the

ZnO/Co<sub>3</sub>O<sub>4</sub> composite allows optimization of the morphology of the ZnO nanorod array to achieve improved photoelectrochemical performance. The results showed that the ZnO/Co<sub>3</sub>O<sub>4</sub> heterostructure exhibited a photocurrent

density of 3.46 mA/cm<sup>2</sup>, while bare ZnO demonstrated a photocurrent density of 0.8 mA/cm<sup>2</sup> at 1.23V. The results of this study provide a better understanding of the mechanism of charge separation and transfer in the heterostructural ZnO/Co<sub>3</sub>O<sub>4</sub> photocatalytic system. Furthermore, the results will be useful for the design and optimization of photocatalytic systems for water splitting and other applications.

#### Keywords

zinc oxide Photoelectrochemistry water splitting cobalt oxide

#### Last published paper details

Aiymkul A. Markhabayeva\*, Zhanar K. Kalkozova, Renata Nemkayeva, Yerassyl Yerlanuly, Assiya A. Anarova, Malika A. Tulegenova, Aida T. Tulegenova and Khabibulla A. Abdullin.Construction of a ZnO heterogeneous structure using Co3O4 as a co-catalyst to enhance photoelectrochemical performance. Materials 2024, 17(1), 146; https://doi.org/10.3390/ma17010146

#### Full title of article

Construction of a ZnO heterogeneous structure using Co3O4 as a co-catalyst to enhance photoelectrochemical performance

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## All authors

Zhanar K. Kalkozova, Renata Nemkayeva, Yerassyl Yerlanuly, Assiya A. Anarova, Malika A. Tulegenova, Aida T. Tulegenova and Khabibulla A. Abdullin

## DOI

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# P.028 Pyrene-functionalized poly(methacrylic acid) acts as an efficient stabilizer for graphene nanoplatelets and facilitates their use in water-borne latex formulations

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#### Abstract

Pyrene end-functionalized poly(methacrylic acid) (Py-PMAA<sub>n</sub>) was prepared by reversible addition-fragmentation chain-transfer (RAFT) polymerization of methacrylic acid using a pyrene-containing RAFT chain-transfer agent (CTA).

graphene nanoplatelet (GNP) dispersions due to the ability of the pyrene end-groups to adsorb to the GNPs and the water solubility of PMAA. These pH responsive Py-PMAA<sub>n</sub> stabilizers performed better than a traditional small molecule surfactant and non-functionalized PMAA. In addition, they were more efficient at high pH due to deprotonation of the carboxylic acid side groups and had improved dispersing ability with increased molecular weight. The use of Py-PMAA<sub>n</sub> allowed GNPs to be readily formulated into water-borne latex coatings, serving as an example of the benefits of using this strategy. The homogeneity of dried nanocomposite films improved when using Py-PMAA<sub>n</sub>, when compared to control experiments and the resulting films were found to be significantly reinforced. Thus, the ability to readily incorporate GNPs into aqueous formulations and enhance GNP/polymer matrix interfaces was demonstrated for these novel amphiphilic stabilizers.

### Keywords

Colloids graphene polymeric surfactant nanocomposite

#### Last published paper details

Yue, Q. et al. (2023) '3D printable, thermo-responsive, self-healing, graphene oxide containing self-assembled hydrogels formed from block copolymer Wormlike Micelles', Soft Matter, 19(34), pp. 6513–6524. doi:10.1039/d3sm00737e.

#### Full title of article

3D printable, thermo-responsive, self-healing, graphene oxide containing self-assembled hydrogels formed from block copolymer wormlike micelles

### Journal

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Soft matter
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#### Year

2023

#### Volume

19

## First page

6513

## All authors

Q Yue, Z Luo, X Li, LA Fielding

## DOI

10.1039/d3sm00737e

# P.029 Designing polyelectrolyte multilayer coatings for enhanced enzyme immobilization on membrane supports to create biomaterials

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## Abstract

Applying polyelectrolyte coatings to commercial filtration membranes is an intelligent approach to introduce specific functional groups onto the membrane surface. This modification facilitates the easier immobilization of enzymes, transforming the entire system into a versatile biomaterial

suitable for various bioapplications, such as sensors and trace compound detectors. This enhanced membrane functionality enables the simultaneous execution of reactions and the efficient separation of target products, expanding its utility across diverse applications. Our study introduces a methodical design for a biocatalytic membrane reactor, involving the integration of physical adsorption and chemical conjugation techniques for Alcohol Dehydrogenase (ADH) within a unique polyelectrolyte (PE) layer-by-layer (LbL) assembly system. The proposed hybrid LbL structure serves as a strategic approach to concurrently enhance the activity and operational stability of enzymes immobilized on a membrane surface. The use of poly(allylamine hydrochloride) (PAH) and poly(methacrylic acid) sodium salt (PMAA) facilitates the functionalization of a polysulfone (Psf) membrane, enabling subsequent ADH immobilization without hindering substrate mass transfer or reducing water permeability (WP) compared to the pristine membrane. By fine-tuning membrane surface chemistry, enzyme concentration, time, and pH during the adsorption process, we achieved an increase in the specific activity of the biocatalytic membrane from 1.13±0.18 mU/cm2 on the pristine membrane to 4.09±0.53 mU/cm2 on a PAH-modified coating. The conjugation of adsorbed ADH with the PMAA layer not only improved reusability, retaining 73.4±3.2% of the initial activity on the third conversion run compared to 58.7±2.4% without conjugation but also shifted the pH optimum by 1 unit compared to free ADH. The presented LbL assembly synthesis approach establishes a promising groundwork for the engineering of nanoscale biocatalytic reactors.

#### Keywords

Membranes Polyeletrolytes Enzyme immobilization

### Last published paper details

Chemical Engineering Science. 285, 10 p., 119638.

#### Full title of article

Comparison of 2D and 3D materials on membrane modification for improved pressure retarded osmosis (PRO) process

#### Journal

**Chemical Engineering Science** 

#### Year

2024

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119638

### All authors

Manuel Pinelo et al.

# P.031 Motion and control of virtual colloidal particles in confined chiral liquid crystals

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<sup>1</sup>University of Barcelona, Spain. <sup>2</sup>Institute of Nanoscience and Nanotechnology of the University of Barcelona, Barcelona, Spain

#### Abstract

Cholesteric phases are liquid crystals in which a helical twist can be induced by the presence of a chiral agent. This twist, with a periodicity or pitch (p), can be frustrated under geometrical confinement comparable to p. Under those conditions, skyrmions can be formed if the material undergoes an instability. Skyrmions are topologically protected solitonic-like structures, formed by the spatial discordance in the orientation of the molecules of the liquid crystal, forming a torus in which the principal axis of the molecules turns 180°. Skyrmions behave as quasi-particles and can be driven by the action of a modulated AC electric field. However, the directionality of their motion has, so far, only been in-situ controlled using complex optical systems. In our work, we study the propulsion of skyrmions under modulated AC electric fields of different amplitude, carrier, and modulation frequencies. Moreover, we also study the collective behaviour of skyrmions, showing different self-assembly regimes in high areal density configurations. We also demonstrate the capability of an external fixed magnetic field to steer driven skyrmions (figure 1 (a)), which can be inserted and controlled within microfluidic channels. Experimental suggest an acceleration when skyrmions are introduced in micro-channels due to distortions in the LC molecular alignment generated by the presence of homeotropic walls (figure 1 (b)). We also show that skyrmions can act as micro-cargo transporters, with a slight modification of their velocity of displacement when loaded.





Figure 1- (a) Motion control of skyrmions under the application of a fixed magnetic field. (b) Skyrmions' acceleration due to the presence of homeotropic walls. Skyrmions' movement is controlled by the application of a fixed magnetic field. In all images, yellow arrows indicate the direction of motion of skyrmions, which is triggered by the application of a modulated AC electric field.

#### Keywords

Cholesteric liquid crystals Active quasi-particles

# P.032 From drop impact to fog harvesting using hydrophobic meshes

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## Abstract

Due to the global water shortage crisis, the demand for water resources intensifies, particularly in Iran, Italy, and China. Extracting water from fog is a promising solution. This research aims to enhance fog collection efficiency by studying the critical factors of surface structure and wettability. Our approach involves creating superhydrophobic meshes through the electrodeposition of copper on steel meshes, followed by a silica-sol modification to boost hydrophobicity. The fabrication strategy imparts to the mesh high surface roughness which, together with the silanization, leads to high advancing and receding contact angles of >145° and >130°, respectively, low hysteresis (<20°), and a sliding angle of <15° for a 2.5 mm drop. Single-drop impact experiments with millimetric drops reveal that while hydrophobicity marginally affects the initial penetration stages, increased hydrophobicity aids in breaking down drops after penetration through the mesh. The result of this study suggests that highly hydrophobic meshes can enhance collection in moderately windy areas  $(1 < U < 2 \text{ m s}^{(-1)})$ . Additional proof-of-concept tests were conducted in a fog chamber, where a microdroplet spray with an average drop diameter of ~ 5-10 µm, generated from a humidifier and mimicking fog, was blown onto the mesh surface mounted at the front of a wind tunnel with  $\sim 0.3$  m s<sup>(-1)</sup> wind speed. The fog collection and the wetting durability of the samples experiments reveal that copper-coated meshes without a silane layer experience clogging, reducing wetting durability and fog collection efficiency which was not observed in single droplet impact experiments. Conversely, copper-coated meshes with an extra silane thin layer demonstrate a fog collection efficiency of ~600 mg/(cm<sup>2</sup> h), marking a 40% improvement compared to an uncoated stainless steel mesh. This advancement holds promise for addressing water scarcity challenges through innovative and efficient fog water harvesting technologies based on surface property design and control.

## Keywords

Surfaces Wetting in liquid-solid interfaces Water collection from fog Hydrophobic mesh

## Last published paper details

F. Cadamuro, M. Ferrario, R. Akbari, C. Antonini, F. Nicotra, L. Russo, Tyrosine glucosylation of collagen films exploiting Horseradish Peroxidase (HRP) ,Carbohydrate Research 533 (2023) 108938

## Full title of article

Tyrosine glucosylation of collagen films exploiting Horseradish Peroxidase (HRP)

## Journal

Carbohydrate Research

## Year

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## All authors

F. Cadamuro, M. Ferrario, R. Akbari, C. Antonini, F. Nicotra, L. Russo

## DOI

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# P.033 Probing active nematics with in-situ microfabricated elastic inclusions

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<sup>1</sup>University of Barcelona, Spain. <sup>2</sup>Institute of Nanoscience and Nanotechnology of the University of Barcelona, Spain. <sup>3</sup>Institute for Bioengineering of Catalonia, Spain

## Abstract

Active nematic dynamics are governed mainly by means of elastic, active and viscous stresses, which reveal the elastic constant (k), activity ( $\alpha$ ) and viscosity ( $\eta$ ) as key parameters of the material. However, the values of these parameters are still unclear. Different approaches have been used to determine them. For example, active nematic viscosity has been studied experimentally and theoretically giving out results with different order of magnitude.

In this work, we present a novel method to determine both the activity and viscosity of active nematic based on force measurements using elastic cantilevers. With a custom DMD-based photolithography technique we are able to build polymeric cantilevers in a microtubule-kinesin based active nematic, from the bottom to the surface. Measuring the deflection of the cantilevers the force applied by the active material can be determined, and then, the force is correlated to the director and velocity fields to obtain the values of the activity and the viscosity of active nematics. The results obtained show that the ratio between activity and viscosity is proportional to the mean vorticity as was previously predicted by Giomi, and the variation of this ratio with the activity follows the trend that was also predicted.

## Keywords

Active nematic activity viscosity hydrogel

## Last published paper details

https://www.mdpi.com/2073-4352/10/2/138

## Full title of article

Stable and Metastable Patterns in Chromonic Nematic Liquid Crystal Droplets Forced with Static and Dynamic Magnetic Fields

#### Journal

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2020

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## All authors

J. Ignés-Mullol, M. Mora, B. Martínez-Prat, I. Vélez-Ceron, R.S. Herrera and F. Sagués

# DOI

10.3390/cryst10020138

# P.034 Cobalt oxide nanocrystal decorated on graphene for secondary air-breathing lithium battery

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# Abstract

Octahedral cobalt oxide  $(Co_3O_4)$  nanocrystals were synthesized onto graphene (GR) nanosheets via hydrolysis and hydrothermal reactions. The  $Co_3O_4$ /GR composite demonstrates improved performance on both oxygen reduction and oxygen evolution capabilities. This catalyst composite was sprayed onto carbon cloth to form a cathode for the hybrid electrolyte lithium-air battery (HELAB). The HELAB was assembled with a lithium metal/organic electrolyte/ceramic lithium-ion conductive membrane/aqueous electrolyte/air cathode configuration and operated at passive, air-breathing mode. These batteries with the developed catalysts demonstrated good long-term stability over 120 hours when fed with high (70-100%) relative humidity ambient air. Futhermore, the results indicated the  $Co_3O_4$ /GR composite in 48.2:51.8 (w/w) is the optimal load for the HELAB due to its balanced amount of catalytic  $Co_3O_4$  and charge-transfer mediated graphene, and good dispersibility of the nanocatalysts on the planar graphene surface.

# Keywords

Metal-air batteries Air cathode Dual electrolyte metal oxide nanocatalyst

# Last published paper details

C.-C. Chen, T.T.V. Truong, S.R. Kumar, C.-C. Hu, D.W. Chen, S.J. Lue\*, Escherichia coli fatality dependence on oxidation level of graphite: Insights into membrane permeabilization and protein leakage, Journal of the Taiwan Institute of Chemical Engineers, 153 (2023) 105194.

# Full title of article

Escherichia coli fatality dependence on oxidation level of graphite: Insights into membrane permeabilization and protein leakage

# Journal

Journal of the Taiwan Institute of Chemical Engineers

## Year

## 2023

## Volume

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# All authors

C.-C. Chen, T.T.V. Truong, S.R. Kumar, C.-C. Hu, D.W. Chen, S.J. Lue

# DOI

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# P.035 Biopesticide formulations for crop protection based on copper oxychloride and a biosurfactant extract from corn industry

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# Abstract

Pesticides are usually incorporated to plants through leaves and roots by directed spray applications, where pesticide formulations play a decisive role in effective crop protection. However, most copper-based pesticides are poorly soluble in water, limiting the availability of copper ions to combat pathogens. Thus, the aim of this work was to develop a copperbased biopesticide (copper oxychloride, Cu-Oxy) by adding a natural and sustainable biosurfactant extract (BS), obtained from a corn stream, in order to improve the effectiveness of Cu-Oxy, for the protection of citrus and tomato leaves. First, the wettability of leaves was evaluated by contact angle measurements using four different solutions: water and Cu-Oxy in water (as controls) as well as BS and Cu-Oxy in BS. Additionally, the surface chemical composition of both leaves was evaluated by X-Ray Photoelectron Spectroscopy (XPS) once treated with the above-mentioned biopesticide formulations and after a water washing process. In general, tomato leaves present a lower contact angle (68.7-77.8°) than citrus leaves (84.9-96.6°), so that the latter are less wettable. Furthermore, Cu-Oxy in BS provides a higher copper content on the surface of both leaves (0.41-0.82%) regarding Cu-Oxy in water (0.16-0.19%), which could be attributed to a higher solubility of Cu-Oxy in the presence of BS. Moreover, the higher Cu content retained on surface of tomato leaves (0.82%) treated with Cu-Oxy in BS regarding citrus leaves (0.41%) confirms that tomato leaves are more wettable (lower contact angle). Finally, the copper content remaining on the surface of two tested leaves after the washing step is considerably higher when using the formulation based on Cu-Oxy in BS (93.3-95.1%) in comparison with the formulation prepared with Cu-Oxy in water (61.3-67.6%). This could be attributed to the fact that the presence of BS could increase the adhesion of copper ions on the leaf surfaces.

# Keywords

copper oxychloride tomato leaves

citrus leaves corn stream

### Last published paper details

Foods 8, 410 (2019)

### Full title of article

A Multifunctional Biosurfactant Extract Obtained from Corn Steep Water as Bactericide for Agrifood Industry

#### Journal

Foods

## Year

2019

# Volume

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1-10

## All authors

A. López-Prieto; X. Vecino; L. Rodríguez-López; A.B. Moldes; J.M. Cruz

# DOI

10.3390/foods8090410

# **P.036** Ecofriendly utilization of spent coffee grounds colloid for the fabrication of superhydrophobic/oleophilic coatings and membranes

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# Abstract

Producing more than 2 million tons of coffee waste per year in Europe is an alarming rate. Repurposing and prolonging the life of this biowaste has been the subject of much research. However, many existing methods involve significant intervention, such as carbonization, chemical modification, or extraction; diverging from green and environmentally friendly practices. Additionally, these methods often overlook the potential to maintain the integrity of the biowaste.

In this work, we present a straightforward and ecofriendly approach to utilize spent coffee grounds (SCG) colloid for the fabrication of superhydrophobic/oleophilic coatings and nanostructured membranes with minimal intervention. The key to our success lies in the ball milling of SCG particles in ethanol, resulting in a highly stable suspension that made all subsequent experiments possible. The fabrication process involves electrospraying the microparticles of SCG to form a coating, followed by a mild activation post-process to achieve a superhydrophobic layer. Additionally, a combination process of electrospraying of SCG and electrospinning of polyacrylonitrile (PAN) nanofibers is used to fabricate a micro-nanoscale membrane. Comprehensive characterization confirms the successful transition of SCG from a hydrophilic substance to a superhydrophobic material, opening up opportunities for various applications, including oil/water separation.

Our approach demonstrates the feasibility of repurposing SCG in an ecofriendly manner, contributing to the broader goals of sustainability and circular economy. By utilizing ethanol

as a green solvent and employing mild post-processing techniques, we advocate for environmentally friendly practices throughout the entire coating process.

## Keywords

Spent Coffee Grounds (SCG) SCG-based colloid Ecofriendly Utilization superhydrophobic/oleophilic

### Last published paper details

https://pubs.acs.org/doi/full/10.1021/acsmaterialsau.3c00025

## Full title of article

Electrospun Poly(vinyl alcohol)-Based Conductive Semi-interpenetrating Polymer Network Fibrous Hydrogel: A Toolbox for Optimal Cross-Linking

#### Journal

ACS Mater. Au

#### Year

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#### Volume

3

### First page

Cross-linking of poly(vinyl alcohol) (PVA) creates a three-dimensional network by bonding adjacent polymer chains. The cross-linked structure, upon immersion in water, turns into a hydrogel, which exhibits unique absorption properties due to the presence of hydrophilic groups within the PVA polymer chains and, simultaneously, ceases to be soluble in

## All authors

Anna Zakrzewska, Shahrooz Zargarian, Chiara Rinoldi, Arkadiusz Gradys, Dariusz Jarząbek, Michele Zanoni, Chiara Gualandi, Massimiliano Lanzi, and Filippo Pierini

## DOI

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# P.037 Computational simulation of the behavior of drug nanoparticles in colorectal cancer tumor tissues

<u>Gustavo Suárez Guerrero</u><sup>1</sup>, Esteban Vallejo Morales<sup>1</sup>, Yvon Maday<sup>2</sup>, Lina Hoyos Palacio<sup>1</sup> <sup>1</sup>Institución Universitaria Pascual Bravo, Colombia. <sup>2</sup>Sorbonne Université, France

## Abstract

According to the World Health Organization (WHO), cancer is one of the leading causes of morbidity and mortality in the world [1]. The most common cases of the disease are breast, lung and colorectal cancer [1]. The therapeutic procedures used for the treatment of cancer are very aggressive, especially chemotherapy, since the drug indiscriminately penetrates and attacks the cellular microenvironment of the whole organism [2]. In this research, mathematical modeling was developed to study the transport of drug nanoparticles in the microenvironment to assess the process of cellular selectivity in the tumor region. Computational models of tumor micromorphology were developed. The biophysical and biochemical
tumor. In the innermost area of the carcinoma, there is high proliferation of the disease, favoring the selectivity process of the nanoparticles with the malignant glands. This research allows for greater understanding of the dynamics between drug nanoparticles and tumor cells to assess therapeutic effectiveness against cancer.

# Keywords

Drug nanoparticles Mathematical modeling Computational simulation Colorectal cancer

#### Last published paper details

World Health Organization. Estimated Number of Incident Cases, Both Sexes, Worldwide (Top 10 Cancer Sites) in 2018; World Health Organization: Geneva, Switzerland, 201 8. Metkar, S.K.; Girigoswami, K. Diagnostic biosensors in medicine —A review. Biocatal. Agric. Biotechnol. 201 9, 17, 271 –283. [Google Scholar] [CrossRef] Liu, Y.; Wu, H.; Zhou, Q.; Song, Q.; Rui, J.; Zou, B.; Zhou, G. Digital quantification of gene methylation in stool DNA by emulsion-PCR coupled with hydrogel immobilized bead-array. Biosens. Bioelectron. 201 7, 92, 596–601 . [Google Scholar] [CrossRef] [PubMed] Oussalah, A.; Rischer, S.; Bensenane, M.; Conroy, G.; Filhine-Tresarrieu, P.; Debard, R.; Forest-Tramoy, D.; Josse, T.; Reinicke, D.; Garcia, M.; et al. Plasma mSEPT9: A Novel Circulating Cell-free DNA-Based Epigenetic Biomarker to Diagnose Hepatocellular Carcinoma. EBioMedicine 201 8, 30, 1 38–1 47. [Google Scholar] [CrossRef] [PubMed][Green V ersion] Song, L.; Jia, J.; Yu, H.; Peng, X.; Xiao, W.; Gong, Y.; Zhou, G.; Han, X.; Li, Y. The performance of the mSEPT9 assay is influenced by algorithm, cancer stage and age, but not sex and cancer location. J. Cancer Res. Clin. Oncol. 201 7, 143, 1 093–11 01 . [Google Scholar] [CrossRef] [PubMed] Lee, H.S.; Hwang, S.M.; Kim, T.S.; Kim, D.W.; Park, D.J.; Kang, S.B.; Kim, H.H.; Park, K.U. Circulating Methylated Septin 9 Nucleic Acid in the Plasma of Patients with Gastrointestinal Cancer in the Stomach and Colon. Transl. Oncol. 201 3, 6, 290–296. [Google Scholar] [CrossRef][Green Version]

#### Full title of article

Computational Simulation of Colorectal Cancer Biomarker Particle Mobility in a 3D Model

#### Journal

Molecules

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#### All authors

Esteban Vallejo Morales, Gustavo Suárez Guerrero, Lina Hoyos Palacio

# DOI

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# P.038 Multi-layering of electrode architectures for boosting charging rates of lithium ion batteries

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#### Abstract

The ability of lithium ion batteries to provide rapid charging characteristics while retaining a substantial energy storage capacity is of paramount significance for their applicability in portable smart electronic devices. In this research, a simple, scalable but relatively unexplored manufacturing approach "spray coating" was utilized to design high mass loading electrodes for use in fast charging and high capacity lithium ion battery applications. A zero-strain intercalation host, namely  $Li_4Ti_5O_{12}$ , and a conductivity booster, namely carbon nanotubes were exploited, which were then assembled as sequential, discrete layers of carbon nanotube-rich  $Li_4Ti_5O_{12}$  and carbon nanotube-free  $Li_4Ti_5O_{12}$ , layer-by-layer, into a single multi-layer electrode architecture, with the aim of promoting recharging rates of lithium ion battery devices while preserving attractive energy storage performance with increasing mass loading in electrodes. Initially, the optimal proportion of a carbon nanotube-rich layer and its best location within multi-layer electrode structures were investigated in half-cell configurations. The best performing multi-layer electrode had an attractive energy-power balance in a full-cell lithium ion battery arrangement that outperformed other combinations of the same active materials. Also, the multi-layer structure was reproduced reliably over  $\geq 20$  cm  $\times 20$  cm current collector areas in a double-sided configuration.

# Keywords

Lithium ion battery Multi-layering fast charging carbon nanotube

# Last published paper details

518-526

#### Full title of article

Multi-layering of carbon conductivity enhancers for boosting rapid recharging performance of high mass loading lithium ion battery electrodes

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# First page

518

All authors

Sang Ho Lee, Yige Sun, Patrick Grant

# P.039 Exploring the functional properties of sodium alginate: A promising coating material for oxygen-sensitive pharmaceutical products

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# Abstract

Pharmaceutical products, including drugs, bioactive compounds, and probiotics, require a high level of protection and often involve controlled release mechanisms. These products, known for their significant health benefits, exhibit heightened sensitivity to oxygen and the acidic environment of gastric juice. Hence, finding a

protecting material capable of shielding them during production, storage and passage through the gastrointestinal tract is crucial. Among various biopolymers. polysaccharides emerge as promising candidates due to their compatibility, availability, and non-toxic nature. This study delves into the investigation of 8 polysaccharides derived from different natural sources (Hydroxypropyl methylcellulose (HPMC), Methylcellulose (MC), Hydroxypropyl cellulose (HPC), Low-methoxyl pectin (LMP), Sodium alginate (SA), Kappa-Carrageenan (KC), Chitosan (CHI) and Pullulan (PUL)) concerning their oxygen and water vapor barrier properties under controlled conditions, in addition to their release behaviors in simulated gastrointestinal fluid (SGF). The findings indicate that SA exhibits outstanding oxygen barrier properties compared to other tested biopolymers. Moreover, owing to the electrophoretic property of SA, its polymer matrix releases only upon entering the intestinal phase, thereby protecting the core materials from the strong acidity in the gastric juice. Further investigations into the functional properties of SA reveal that the molecular weight and the ratio of guluronic and mannuronic blocks in SA chains do not impact the barrier properties of SA films. However, these characteristics significantly influence the release behavior of the SA matrix in SGF. Therefore, tailoring these molecular specifications of SA could facilitate the targeted delivery of core materials to different locations within the gastrointestinal tract. In conclusion, SA emerges as an excellent candidate for use as a protective material, ensuring both the protection and colonic administration of pharmaceutical products.

#### Keywords

Sodium alginate barrier properties colonic delivery functional properties

# Last published paper details

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# Full title of article

Comprehensive approach to the protection and controlled release of extremely oxygen sensitive probiotics using edible polysaccharide-based coatings

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# All authors

Thị-Thanh-Trúc Phùng, Massimiliano Gerometta, Julie Chanut, Audrey Raise, María Ureña, Sébastien Dupont, Laurent Beney, Thomas Karbowiak

# DOI

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# P.040 Suspensibility of agrochemical active ingredients in the presence of biosurfactants produced at pilot-scale

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# Abstract

Suspensibility is an important property of agrochemicals, as many pesticides are commercially available as dispersible granules or wettable powders and they are applied to crops in form of homogeneous spraying suspensions. Furthermore, the stability of these suspensions significantly affects their effectiveness against plant pathogens. The Food and Agriculture Organization of the United Nations (FAO) recommends that the suspensibility of active ingredients in pesticides should not be below 60% after 30 min. Nevertheless, this property can be improved by reducing the particle size of solid products and by adding surfactants to commercial formulations. In this sense, the corn steep liquor (CSL), a residual stream of corn milling industry, can be considered an effective source of biosurfactants (BS) with diverse applications. Accordingly, in this work it was evaluated the influence of three synthetic surfactants (CTAB, SDS and Tween-20) and three CSLbiosurfactants (BS1, BS2 and BS3) on the suspensibility of two active ingredients widely employed in agrochemical applications: copper oxychloride (Cu-Oxy) and cuprous oxide (Cu-Ox). The CIPAC (Collaborative International Pesticides Analytical Council) MT 184-1 protocol, slightly modified, was employed to assess their suspensibility in water. The content of Total Suspended Solids (TSS) was gravimetrically determined by means of UNE-EN 872 protocol. Furthermore, a more simplified analytical procedure was developed by establishing a linear correlation between TSS content and turbidity measurements in Nephelometric Turbidity Units (NTU) using kaolin G-30 M. The results obtained indicate that BS2 and synthetic surfactants gave suspensibility values between 14.74%-25.61% for Cu-Oxy and between 7.23%-12.24% for Cu-Ox. In contrast, biosurfactants B1 and B3 provided much less stable suspensions, with suspensibility values always below 9.27%.

# Keywords

suspensibility pesticides surface-active compounds corn stream

# Last published paper details

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Fungicide Effect of a Novelty Antimicrobial Biosurfactant Extract Alone or Combined with Copper Oxychloride on Botrytis cinerea Cells

#### Journal

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2023

# Volume

9

# First page

1-14

# All authors

A. López-Prieto, A.B. Moldes, J.M. Cruz and B. Pérez-Cid

# DOI

10.3390/fermentation9060528

# **P.041** Ionic strength-induced compartmentalization in poly(*n*-isopropylacrylamide) and poly(acrylamide) nanogel-in-microgel colloids

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# Abstract

The need for compartmentalization in microgels has surged in fields like drug delivery, catalysis and microrobotics, enabling the incorporation of multiple different materials, functionalities and properties. In droplet-based microfluidics, the fabrication of microgels with multiple compartments is achieved via multiple emulsions or induced phase separation from homogeneous droplets.<sup>[1]</sup> Previously, the latter was realized with e.g. temperature increase or UV irradiation.<sup>[2]</sup> However, these methods are restricted to specific systems and prevent the incorporation of sensitive (biological) cargo. This work circumvents these limitations by introducing ionic strength-induced compartmentalization in nanogel-in-microgel colloids (NiM-C). Precipitation polymerization was used to synthesize smaller neutral, negatively, and positively charged poly(Nisopropylacrylamide) (PNIPAAm) based microgels. These are around 500 nm in diameter and here termed "nanogels" for better differentiation. Subsequently, these nanogels were incorporated into larger microgels (around 150 µm) based on either PNIPAAm or poly(acrylamide) (PAAm) through microfluidics. The ionic strength of the solution containing monomers and nanogels was adjusted on-chip using a second aqueous phase with varying sodium chloride concentrations (0 mM -2000 mM). This led to precipitation of the nanogels inside the microfluidic droplets due to hydrophobic interactions. The hereby-formed compartments were immobilized through UV-initiated polymerization of the monomer species. Upon ionic strength optimization, compartmentalization was realized for all NiM-C compositions as confirmed with confocal laser scanning microscopy. Notably, the PAAm NiM-C exhibited anisotropic shape changes as the compartments changed in size depending on the temperature, while the surrounding network maintained consistent dimensions across the investigated temperature range. The anisotropic shape change has potential for the development of microbots or controlled drug delivery systems.

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#### Keywords

Microgels Anisotropy Temperature responsiveness

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Hannah F. Mathews, Maria I. Pieper, Se-Hyeong Jung, Andrij Pich, Compartmentalized Polyampholyte Microgels by Depletion Flocculation and Coacervation of Nanogels in Emulsion Droplets, Angewandte Chemie International Edition, 62, 36, e202304908

# Full title of article

Compartmentalized Polyampholyte Microgels by Depletion Flocculation and Coacervation of Nanogels in Emulsion Droplets

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#### All authors

Hannah F. Mathews, Maria I. Pieper, Se-Hyeong Jung, Andrij Pich

# DOI

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# P.042 Selected composites of green clay, hydroxyapatite, silica, TiO2, ZnO and spirulina or *Clitoria Ternatea L.*

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# Abstract

Clays are one of the most promising nanomaterials. They owe their popularity primarily to low costs, high stability and biocompatibility. One of the most commonly used clays is green clay, where the main ingredient is montmorillonite. It is a layered material composed of aluminosilicate plates separated by layers of water (2:1) [1]. Hydroxyapatite is the main mineral building block of bones and teeth. In composites, hydroxyapatite nanoparticles have broad stabilizing abilities [2].

The characteristics and stability of nanoparticles depend largely on environmental conditions such as pH, ionic strength, ionic composition and temperature, as well as on co-existing colloids. Colloids have great potential to interact with nanoparticles. Interaction and association can influence the stability and behavior of molecules. Since organic and inorganic colloids often coexist, further research is needed on the effects of colloids with different properties and their impact on the stability of nanoparticles [3].

The analysis of composites synthesized for future cosmetic purposes was performed on the basis of selected analyzes characteristic of this type of nanomaterials. These include tests such as toxicity assessment, determination of the concentration of anthocyanins, chlorophyll and carotenoids, particle size measurements and surface analysis, and electrokinetic properties.

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# Keywords

Green clay Hydroxyapatite Spirulina Clitoria Ternatea L.

#### Last published paper details

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# Full title of article

Research on deposition of silver nanoparticles at the cellulose/NaNO3 electrolyte interface

# Journal

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# All authors

W. Janusz, K. Kowalska, E. Skwarek

# DOI

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# P.043 Development of CuO/ $Cu_4(OH)_6SO_4$ nanoparticle mixtures to optimise the H2S adsorption

Donald Hill, Yubiao Niu, Omotoke Olonisakin Olonisakin, Henry Apsey, Richard E. Palmer, Shirin Alexander Swansea University, UK

# Abstract

This study investigates the hydrogen sulfide adsorption behaviour of a novel nanocomposite material, formed from a mixture of copper(II) oxide (CuO) and brochantite  $(Cu_4(OH)_6SO_4)$  nanoparticles. Hydrogen sulfide  $(H_2S)$  gas is a malodorous, corrosive pollutant with a distinctive "rotten egg" smell. It is produced from a number of natural and anthrophogenic sources, and is found in high concentrations in oil and gas wells where its toxicity poses a risk to life, as well as in wastewater treatment facilities where it is produced as a by product of anaerobic digestion. In addition, catalysts used to carry out the hydrogen

readily prepared through the room temperature addition of NaOH<sub>(aq)</sub> to CuSO<sub>4 (aq)</sub> and contain particles with wire-like morphologies that can be less than 10 nm in thickness but hundreds of nanometres in length, as observed using scanning transmission electron microscopy. The high aspect ratio that these cupric particles possess makes them highly reactive towards chemisorption of H<sub>2</sub>S, which is shown when they are deposited onto polymer foams to make highly effective filters for the gas. Breakthrough experiments indicate that the particles' functional interface can be utilised as a sorbent that shows performance that is over an order of magnitude greater than commercially available CuO and other materials that have been reported as having significant H<sub>2</sub>S adsorption efficacy, such as Fe<sub>2</sub>O<sub>3</sub> or activated charcoal. The high reactivity of these particles, along with their synthetic ease of production, could make them suitable for use in situations where high levels of H<sub>2</sub>S poses a problem, such as in protective clothing articles, or for application onto filter media in the medical sector.

# Keywords

nanowire hydrogen sulfide nanocomposite malodour

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Development of CuO/ Cu4(OH)6SO4 nanoparticle mixtures to optimise the H2S adsorption

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# All authors

Donald Hill, Yubiao Niu, Henry Apsey, Omotoke Olonisakin, Richard Palmer and Shirin Alexander

# DOI

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# P.044 The role of colloidal nanobubbles in the anti-solvent crystallization of glycine.

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# Abstract

Nanobubbles are nanoentities possessing distinctive features including a high surface-tovolume ratio, efficient gas mass transfer, high laplace pressure, and extraordinary longevity. Due to these unique properties, they have been highly utilized in various applications like waste-water treatment, mineral flotation, etc. Recent studies have revealed the incorporation of these bubbles in the crystallization processes. Although crystallization is one of the oldest and most efficient separation techniques, many challenges, including inefficient mixing, high energy consumption, poor uniformity, and scale-up, have not been addressed. Several attempts, like sono-crystallization, microfluidic-based crystallization, etc., have been made towards optimization. However, greener and more energy-efficient technology with easy scaling is required.

In the current work, glycine has been crystallized using anti-solvents such as methanol, ethanol, isopropanol, and acetone in the presence of nanobubbles created from different gases like nitrogen, oxygen, and argon, with crystallization times of 1 min and 5 min. The porous membrane method was used to generate nanobubbles of different gases with a mean size of 150–250 nm, a strong negative charge of -29 mV to -36 mV, and a high concentration of  $10^7$  in the saturated glycine solution. The results indicated that nucleation occurred at a faster rate without any external energy requirements. It was found that the crystal size was seen to increase, whereas the specific surface area decreased with the addition of nanobubbles to the glycine solution treated with methanol. In the instance of ethanol, the specific surface area increased by 32% and the crystal size decreased by 33% in the presence of nanobubbles. It was also noted that the presence of nanobubbles resulted in more uniform crystals with the formation of  $\alpha$ -polymorph. According to the findings, the existence of nanobubbles may be able to regulate the crystallization process and provide effective homogeneous mixing of the antisolvent and solute.

# Keywords

Bulk Nanobubbles Nucleation Anti-solvent Glycine

# Last published paper details

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# Full title of article

Thermal energy storage in a confined cylindrical heat source filled with phase change materials.

# Journal

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### First page

Thermal energy storage in a confined cylindrical heat source filled with phase change materials Aakriti Sharma, Mohit Trivedi, Kalyani Agarwal, Neelkanth Nirmalkar\* Department of Chemical Engineering, Indian Institute of Technology, Ropar 140001, India

#### All authors

Aakriti Sharma, Mohit Trivedi, Kalyani Agarwal, Neelkanth Nirmalkar.

#### DOI

https://doi.org/10.1016/j.ijheatmasstransfer.2021.121603

# P.045 Aromatization of aliphatic hydrocarbons over HZSM-5

Barbora Grycova, Katerina Klemencova, Amer Inayat, Pavel Lestinsky VSB -Technical University of Ostrava, CEET, IET, Czech Republic

#### Abstract

Hydrocarbons can be converted into more valuable products through the process of aromatization, which involves the transformation of aliphatic compounds into aromatic compounds. The reaction involves the conversion of straight-chain or branched-chain alkanes into aromatic compounds, such as benzene, toluene, and xylene. The selectivity and yield of the aromatization process depend on several factors, including the nature of the hydrocarbon feedstock, the reaction conditions, and the properties of the catalyst. One of the catalysts commonly used for this process is HZSM-5, which is a zeolite with a high concentration of Brønsted acid sites. Besides that, the pore structure of the zeolite helps to shape selectively convert the molecules into the desired products. However, the easy deactivation of microporous HZSM-5 due to carbon deposition complicates the aromatization of light hydrocarbons by limiting the mass transfer of both reactants and products inside the micropore. To overcome these issues, the hierarchical HZSM-5 with both a micropore and mesopore structure has been proposed to improve its catalytic performance.

In our recent work, investigation of virgin polyolefins thermo-catalytic pyrolysis over HZSM-5 zeolite catalysts considering the influence of catalyst acidity, operation mode and process parameters was reported. The present work is a follow-up study of n-pentane, n-hexane, cyclohexane, n-octane, iso-octane, etc. aromatization reactions performed in a reactor with ex-situ catalyst heated up to 500 °C using heating rate of 10 °C/min. The results will help to understand the processes involved in the thermo-catalytic pyrolysis of polyolefins.

Experimental results were accomplished by using financial support of the European Union under the REFRESH -Research Excellence For REgion Sustainability and High-tech Industries project No. CZ.10.03.01/00/22\_003/0000048 via the Operational Programme Just Transition and Large Research Infrastructure - Energy Waste Recovery and Gas Treatment supported by the Ministry of Education, Youth and Sports of the Czech Republic under Project Number LM2023056.

#### Keywords

Catalytic cracking Hydrocarbons Aromatization HZSM-5

#### Last published paper details

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# Full title of article

Conductivity of carbonized and activated leather waste

#### Journal

Sustainable Chemistry and Pharmacy

Year

2023

#### Volume

35

#### First page

The conductivity of chromium-tanned pigskin leather waste carbonized in various manner to nitrogen-containing carbons is reported. Four protocols have been tested: The simple carbonization at 800 °C in inert atmosphere, the carbonization at 500 °C followed by the activation with potassium hydroxide at 800 °C, etc.

#### All authors

Barbora Grycová a, Kateřina Klemencova, Pavel Lestinsky, Jaroslav Stejskal, Tomas Saha, Miroslava Trchova, Jan Prokes

# P.046 Experimental study of catalytic pyrolysis of waste polypropylene over HZSM-5

<u>Katerina Klemencova</u>, Barbora Grycova, Pavel Lestinsky, Amer Inayat VSB-TUO, CEET, IET, Czech Republic

#### Abstract

Humans have already produced more than eight billion tons of plastic. Half of the 8.3 billion tons was produced in the last 13 years. If things continue like this, 34 billion tons of plastic will be created by the middle of the 21st century. Currently, most plastics ever produced end up in landfills. Due to their durability it remains in environment. Plastic waste as of the most promising resources can be converted into valuable products which can be used as secondary feedstocks in chemical and petrochemical industries.

Zeolites have proven to be successful catalysts in the degradation of polypropylene into light hydrocarbons. HZSM-5 zeolite is one widely used catalyst, given its strong acidity and shape selectivity, which depends on the particular textural properties, structure and pore size of this catalyst. HZSM-5 was used for catalytic depolymerization. The effect of temperature and catalyst on product distribution in PP pyrolysis was monitored. Thermal and thermo-catalytic depolymerization of PP was carried out including the possibility of catalyst reusing. The temperature range between 450 °C and 550 °C, heating rate of 10 °C/min and residence time of 30 minutes were used for all experiments. The catalytic pyrolysis created 60 wt% of pyrolysis oil which was contained mainly by BTEX group. The amount of gas composed of C<sub>1</sub>-C<sub>4</sub> Alkanes. The results show that the regenerated catalyst had the same efficiency as the original catalyst.

Experimental results were accomplished by using financial support of the European Union under the REFRESH -Research Excellence For REgion Sustainability and High-tech Industries project No. CZ.10.03.01/00/22\_003/0000048 via the Operational Programme Just Transition and Large Research Infrastructure - Energy Waste Recovery and Gas Treatment supported by the Ministry of Education, Youth and Sports of the Czech Republic under Project Number LM2023056.

# Keywords

Waste polymers, Pyrolysis Catalysis Zeolite

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# Full title of article

Chemical recycling of waste polypropylene via thermo-catalytic pyrolysis over HZSM-5 catalysts.

#### Journal

**Chemical Engineering Technology** 

Year

2023

#### Volume

46

# First page

The present work deals with the chemical recycling of waste polypropylene via thermocatalytic pyrolysis over HZSM-5 zeolite catalysts. The main aim was to systematically investigate the influence of reactor configuration, zeolite acidity, polypropylene wastes, obtained from different sources, as well as catalyst regeneration on the product distribution.

# All authors

Inayat A, Inayat A, Schwieger W, Klemencova K, Lestinsky P.

# DOI

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# P.047 Coupling SMLS analysis and the HLD approach to assess the amphiphilicity of surfactants

<u>Guillaume LEMAHIEU</u>, Matthieu Bouzaid Microtrac - Formulaction, France

#### Abstract

The selection of the most effective surfactants for a target application requires an accurate knowledge of their behavior in complex environments. This is especially true for detergent and Home & Personal Care (HPC) formulations that must remain effective in a wide range of salinity and temperature conditions. In such applications, surfactants are used to decrease the interfacial tension between fats and tap water down to low values for ensuring an efficient cleaning mechanism. However, salinity and temperature variations can really inhibit the surfactant affinity for interface and induce a loss of efficiency. It is particularly the case for ionic surfactants which tend to precipitate with the increase of salinity by charge screening, or for nonionic ones which become insoluble with the increase of temperature by dehydration. To prevent such problematics, the salinity and temperature sensibility of surfactant need to be known. In this work, we use the Static Multiple Light Scattering (SMLS) analysis in conjunction with the HLD concept to unambiguously evaluate the salinity resistance, the temperature sensitivity and the oil compatibility of surfactants. To characterize surfactants, the SMLS analysis has been adapted to identify efficiently the WIII microemulsion conditions through the phase inversion detection at different temperatures during a continuous aqueous salinity variation in model emulsions under stirring. Using a well-described surfactant as reference, this experimental method allows the estimation of three parameters derived from the HLD equation ( $\delta_{S}$ ,  $\delta_{T}$  and PACN) representative of the salinity resistance, the temperature sensitivity and the oil compatibility of unknown surfactants under study. Using a such characterization allows to choose the best surfactants to use in function of salinity and temperature working conditions. Accordingly, this characterization technique appears to be a major step toward the rapid screening of surfactants for adaptability in detergent and HPC formulations, with numerous applications in reformulation.

#### Keywords

Surfactants HLD SMLS Salinity

#### Last published paper details

SENTIS, Matthias PL, LEMAHIEU, Guillaume, HEMSLEY, Elizabeth, et al. Size distribution of migrating particles and droplets under gravity in concentrated dispersions measured with static multiple light scattering. Journal of Colloid and Interface Science, 2024, vol. 653, p. 1358-1368.

#### Full title of article

Size distribution of migrating particles and droplets under gravity in concentrated dispersions measured with static multiple light scattering

#### Journal

Journal of Colloid and Interface Science

#### Year

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#### All authors

Matthias P.L. Sentis, Guillaume Lemahieu, Elizabeth Hemsley, Matthieu Bouzaid, Giovanni Brambilla

# DOI

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# P.048 Carbon dots from perylenetetracarboxylic dianhydride for supercapacitor application

Dhanya Sunil, Namratha Ullal

# Abstract

Carbon dots (CDs) are prepared from Perylenetetracarboxylic dianhydride via hydrothermal approach and purified using column chromatography. Among the five fractions separated, a polymer electrolyte was prepared using the third fraction CDs with sodium alginate (SA), and MgCl<sub>2</sub> for potental use in energy storage application. A supercapacitor was fabricated and tested for its electrochemical performance such as cyclic voltammtery (CV), electrochemical impedance spectroscopy (EIS) and galvonastatic charge/discharge studies (GCD). The comparsion of CVs of pure SA, SA/CD and SA/CD/Mg showed an enhanced current window for SA/QD than the other two films which indicates a structural interaction of CD with SA. The dual ionic interaction of sodium and Mg along with enhanced structural stability due to doped QD makes it convenient for supercapacitor application. The fabricated supercapacitor showed a specific capacitance of 84 F/g. The GCD of the device shows pseudocapacitance behaviour and quiet stable for 2000 cycles with coulombic efficiency of 96%.

# Keywords

Carbon dots purification supercapacitor

# Last published paper details

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# Full title of article

Fluorene-naphthalene Schiff base as a smart pigment in invisible ink with multiple security features for advanced anticounterfeiting and forensic applications

#### Journal

Journal of Colloid And Interface Science

Year

2024

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653

#### First page

Smart functional materials with captivating optical properties are of immense importance due to their versatile applicability in anticounterfeiting and forensic science. A fluorene-naphthalene Schiff base (FNH) that displays aggregation induced emission, mechanofluorochromism and excitation wavelength dependent fluorescence inherent to the pristine and ground samples is synthesized.

#### All authors

Kashmitha Muthamma, Sudarshan Acharya, Dhanya Sunil, Prakasha Shetty, Abdul Ajees Abdul Salam, Suresh D Kulkarni, Anand P J

# DOI

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# P.049 Gelatin-based porous hydrogel foams for controlled adsorption and release of drugs

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# Abstract

Gelatin is an abundant biomolecule which has been used as a building block for artificial tissues or drug delivery systems [1]. For a better processability, gelatin is often chemically modified to change the gelling behavior and to lower the viscosity of its solutions. Modifications with ionic groups also change the isoelectric point (IEP) of gelatin, thus introducing an additional parameter to control drug release. Concomitant modification with methacryl groups allows the photochemical crosslinking of the gelatin derivatives. Bulk hydrogels are obtained by pouring the solution into a mold, followed by crosslinking. However, these hydrogels have a small surface, which is disadvantageous for drug release. A more sophisticated way is to use foam templating [2-4] where the gelatin solution is first foamed and then crosslinked, yielding a porous hydrogel with a large surface. Microfluidics provide control of the bubble size and the bubble size distribution and thus foams with well-defined structures [2-4].

This work aims to produce gelatin-based porous hydrogels with a large range of IEPs and well-defined structures for drug release studies. We present the first steps toward such materials, namely (1) the synthesis and characterization of two gelatin derivatives GM10 (IEP = 4.1) and GM10E10 (IEP = 9.5), (2) the mixing of the derivatives to adjust the IEP between 4.1 and 9.5, (3) the foaming of the derivatives and their mixtures, and (4) the generation of porous hydrogels with pore radii of 250 - 450  $\mu$ m.



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[1]	Su et al. Biotechnology Letters 2015, 37, 2139.
[2]	Dehli <i>et al. Biomacromolecules</i> <b>2019</b> , <i>20</i> , 2666.
[3]	Dehli et al. Journal of Colloid and Interface Science 2021, 588, 326
[4]	Dehli <i>et al. Macromolecular bioscience</i> <b>2022</b> , 22, e2200139.

Keywords

Porous hydrogel foams Modified gelatin Foam templating Microfluidics

#### Last published paper details

-

## Full title of article

Influence of a CO2-switchable additive on the surface and foaming properties of a cationic non-switchable surfactant

#### Journal

Soft Matter

# Year

2023

# Volume

19

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2941

# All authors

Robin R. Benedix; Sophia Botsch, Natalie Preisig; Volodymyr Kovalchuk; Philip Jessop; Cosima Stubenrauch

DOI

10.1039/D3SM00273J

# P.050 Advanced 3D-printed bis-picolyamine based-adsorbent: Efficient solution for selective recovery of Cu (II) from wastewater and tailings

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# Abstract

Copper is a critical metal frequently present in elevated concentrations in wastewater and tailings due to its widespread use in various industries. Implementing selective copper recovery from secondary resources offers a valuable source of copper. Chelating resins with bis-picolylamine functional groups are suitable for this purpose, but their small particle size poses challenges in their handling and recycling. Combining 3D printing technology with chelating resins emerges as a promising solution. This study focuses on developing and evaluating a 3D-printed porous adsorbent functionalized with bis-picolyamine groups for selective copper recovery from copper tailings. The characterization of the 3D-printed adsorbent was performed by FTIR, SEM, and zeta potential, and its adsorption behavior under varying conditions, including the kinetics and isotherm studies, were examined. The results indicated a favorable fit to Langmuir isotherm models and pseudo-second-order kinetics, suggesting monolayer and chemical adsorption. FTIR studies suggested coordination interaction as a potential adsorption mechanism, and thermodynamic analyses revealed an endothermic process. The 3D-printed adsorbent exhibited excellent Cu(II) adsorption efficiency, reusability, and high selectivity, showing its

potential for selective Cu(II) recovery and addressing challenges in particle handling, ease of use, and separation from real industrial application.

# Keywords

3D-printing Adsorption bis-picolylamine copper

#### Last published paper details

K. Ibebunjo, Y. El Ouardi, J. Kwame, A. lurchenkova, E. Repo, Functionalization of recycled polymer and 3D printing into porous structures for selective recovery of copper from copper tailings, Chem. Eng. Sci. 286 (2024) 119664. https://doi.org/10.1016/j.ces.2023.119664.

# Full title of article

Functionalization of Recycled Polymer and 3D printing into Porous Structures for Selective Recovery of Copper from Copper Tailings

#### Journal

Chemical engineering science

#### Year

2024

#### Volume

286

# First page

1

# All authors

K. Ibebunjo, Y. El Ouardi, J. Kwame, A. lurchenkova, E. Repo

# **P.051** Evolution of functionalized nanomaterials from surface chemical modification to membrane encapsulation

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# Abstract

A simple case demonstrates amino acids-modified Au@Cu2O nanoparticle to act as a catalysis-mediated biosensor, enabling the detection of the trace keto acids. Even though the mature surface chemical modification endows the various additional functions of specific nanomaterials, the inevitable risk of these nanomaterials injected into the body is to cause a robust immune response and potential toxicity. Advanced nanomaterials regarding extracellular vesicles (EVs) and membrane-camouflaged nanoparticles showing significant advantages and potential in various biomedical applications lead a bright direction. However, the poor yield of natural EVs has greatly restricted related developments. A practical approach, termed liposome fusion-induced membrane exchange (LIME), was established by feeding an excess highlyfluid liposome to the exoelectrogenic bacteria (Shewanella oneidensis MR-1), thereby producing the biomimetic EVs with abundant electroactive c-type cytochromes (c-Cyts) in milligram quantities. These electroactive EVs were applied to coat on the membrane play a vital role as an electron channel in facilitating charge mobility, revealing the great potential to improve the intrinsic properties of nanocomposites.

# Keywords

liposome surface chemical modification extracellular electron transfer membrane-coated nanoparticle

#### Last published paper details

Dynamic therapies have potential in cancer treatments but have limitations in efficiency and penetration depth. Here a membrane-integrated liposome (MIL) is created to coat titanium dioxide (TiO2) nanoparticles to enhance electron transfer and increase radical production under low-dose X-ray irradiation. The exoelectrogenic Shewanella oneidensis MR-1 microorganism presents an innate capability for extracellular electron transfer (EET). An EET-mimicking photocatalytic system is created by coating the TiO2 nanoparticles with the MIL, which significantly enhances superoxide anions generation under low-dose (1 Gy) X-ray activation. The c-type cytochromes-constructed electron channel in the membrane mimics electron transfer to surrounding oxygen. Moreover, the hole transport in the valence band is also observed for water oxidation to produce hydroxyl radicals. The TiO2@MIL system is demonstrated against orthotopic liver tumours in vivo.

#### Full title of article

Electroactive membrane fusion-liposome for increased electron transfer to enhance radiodynamic therapy.

#### Journal

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#### Year

2023

#### Volume

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#### First page

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# All authors

Ying-Chi Chen, Yi-Ting Li, Chin-Lai Lee, Yen-Ting Kuo, Chia-Lun Ho, Wei-Che Lin, Ming-Chien Hsu, Xizi Long, Jia-Sin Chen, Wei-Peng Li, Chia-Hao Su, Akihiro Okamoto & Chen-Sheng Yeh

# DOI

10.1038/s41565-023-01476-2

# P.052 Aggregation of small molecules induces the inhibition of DNase I

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# Abstract

Streptococcal toxic shock syndrome is a serious disease with a fatality rate of more than 30%. Neutrophil eliminates pathogens by releasing neutrophil extracellular traps (NETs) composed of their genome DNA. *Streptococcus pyogenes*,

agent for streptococcal infections by inhibiting the DNase secreted by streptococci. To specify the key structure in Mn007 for the inhibition of DNase I, we divided the structure of Mn007 into parts, and investigated their DNase inhibitory effect of each part. Each part was conjugated with a long alkyl chain to maintain the aggregation property in an aqueous solution.

Compound 1 (Comp.1) was synthesized by introducing an alkyl chain to the thiophene ring-containing substructure of Mn007. The critical aggregation concentration (CAC) of Comp.1 was determined to be  $9.7 \mu$ M. Comp.1 inhibited DNase I above its CAC, which meant that the aggregation of Comp.1 was necessary to inhibit DNase I, being similar to Mn007. Thus, we figured that the substructure of Mn007 used for Comp.1 plays an essential role for the DNase I inhibition. To control the availability and the aggregation size of Comp.1, we integrated Comp.1 on liposomes. We synthesized Comp.1 derivatives having various lengths of alkyl chains and prepared liposomes composed the derivatives and phospholipids. The inhibitory effects of the derivatives will be reported in the poster presentation.

# Keywords

Self-assembly
Enzyme
Inhibition
Biomimetic membrane

# Last published paper details

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Full title of article

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DOI

N/A

# P.053 Enhancement in electrical conductivity of ZnO doped H-bonded liquid crystals

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# Abstract

Currently, the composites of liquid crystals with nanoparticles are the front runners in soft matter studies. The intriguing interest in this field arises from the fact that a drastic change in the behavior/properties of liquid crystals is realized upon their interaction with nanoparticles. Herein, nanoparticle-doped liquid crystal composites involving noncovalent forces are prepared, and their

crucial life-sustaining water molecules all possess the hydrogen bonds. The synthesis of liquid crystals involving hydrogen bonds is more sustainable as it involves non-corrosive chemicals and solvents in minimum quantities. The process is a simple single step condensation reaction with elimination of water molecules. The synthesized compounds are water soluble and thus contribute to the principles of green synthesis. Zinc oxide nanoparticles (ZnO NPs) of 118nm particle size were synthesized using a simple starting material. The hydrogen bonded liquid crystal (HBLC) built from acid moieties and Schiff bases of varying carbon chain lengths (octyl and octadecyl), were used as the host, and ZnO nanoparticles were doped into them. The nanocomposites thus obtained displayed enhanced conductivity. This type of LCs is useful for displays, optical fibers and sensors.

# Keywords

Hydrogen bonded liquid crystals ZnO nanoparticles conductivity green synthesis

# Last published paper details

The plinths of hydrogen-bonding in liquid crystals: Carboxylic acids as proton donors to emphasize on the hydrogen bonding in liquid crystals, Journal of Molecular Structure, 2024, 1301, 137367

# Full title of article

The plinths of hydrogen-bonding in liquid crystals: Carboxylic acids as proton donors to emphasize on the hydrogen bonding in liquid crystals

#### Journal

Journal of Molecular Structure

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□ Alkyl/Alkyloxy benzoic acids are reviewed as proton donors in various hydrogen-bonded supramolecules. □ Contributions of non-mesogenic substituted benzoic acids in influencing mesomorphism are deliberated. □ The influence of alkyl/alkyloxy chains of the acids and different electron-withdrawing substituents of the acids contributing to mesomorphism is discussed.

# All authors

Sonali M K, Rajeev K Sinha, Suresh D Kulkarni, Poornima Bhagavath\*

# DOI

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# P.054 Enhancing surface functionalization stability through crosslinking: Impact of adsorbed fatty acids on metal surfaces

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# Abstract

Surface functionalization is a process of altering the surface properties by introducing specific functional molecules, thus developing the materials that differ from original. The preparation of a homogeneous and organized layer of molecules on a substrate is crucial for surface functionalization. Once the layer is prepared, it must remain stable and durable on the surface. Cross-linking the molecules attached to the surface to form a polymer coating will significantly improve the durability. However, the cross-linking must also be homogeneous so that the coating remains stable, without weak points where the coating can detach from the surface. Cross-linking can be successfully achieved by ionizing irradiation under suitable conditions [1]. It is expected that the structure of the long-chain molecules applied to the surface is expected to influence both the layer formation and the cross-linking process. In the case of crosslinking, a double bond in the molecular structure is supposed to serve as the crosslinking center.

In order to investigate the influence of the molecular structure on the successful formation of a polymer film, three types of fatty acids were applied to the copper surface. All applied molecules consist of 18 carbon atoms. Two fatty acids are unsaturated with a double bond at the  $C_9$  position.

In the case of elaidic acid, the double bond is in the *trans* position, while in the case of oleic acid it is in the *cis* position. The unsaturated fatty acids were compared with a saturated fatty acid, stearic acid. The resistance of the layers was analyzed under simulated atmospheric conditions and using various electrochemical techniques, while the surface was characterized by AFM, FTIR, ellipsometry and contact angle measurements.

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[1] Small 19/30 (2023) 2301104.

#### Keywords

surface functionalization radiation induced cross-linking fatty acids polymer nanocoatings

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#### Full title of article

Green Nanocoatings Prepared by Crosslinking Self-Assembled Fatty Acids on Metals

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# All authors

K. Marušić, E. Pezić, N. Matijaković Mlinarić, P. Dubček, J. Sancho-Parramon, D. Kralj, B. Mihaljević

# DOI

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# **P.055** Tuning wetting-dewetting thermomechanical energy for hydrophobic nanopores: Preferential intrusion

<u>Luis Bartolomé</u><sup>1</sup>, Argyrios Anagnostopoulos<sup>2</sup>, Alexander R. Lowe<sup>2</sup>, Piotr Ślęczkowsk<sup>2</sup>, Eder Amayuelas<sup>1</sup>, Andrea Le Donne<sup>3</sup>, Michał Wasiak<sup>4</sup>, Mirosław Chorążewski<sup>2</sup>, Simone Meloni<sup>3</sup>, Yaroslav Grosu<sup>1</sup>

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<sup>3</sup>Università degli Studi di Ferrara, Italy. <sup>4</sup>University of Łódź, Poland

# Abstract

The thermomechanical energy of compression/decompression, which is relevant to many industrial and natural processes, is a prominent property of thermodynamic systems. Unfortunately, this property is challenging to tune due to fundamental limitations for simple fluids. However, in this presentation, we demonstrate via direct experimental and atomistic observations that these fundamental limitations can be overcome by exploiting the preferential intrusion of water from aqueous solutions into sub-nanometer pores. This strategy is demonstrated for heterogeneous systems consisting of a lyophobic porous material and a non-wetting liquid subjected to intrusion-extrusion phenomenon. Moreover, during this intrusion-extrusion process, i.e. when compression/decompression pressures are sufficient to push/release the liquid into/from nanopores, both thermal and mechanical energies of compression/decompression are noticeably affected. We hypothesize that this effect is due to the enthalpy of dilution manifesting itself as the aqueous solution concentrates upon the preferential intrusion of pure water into the pores. Therefore, we suggest that this genuinely sub-nanoscale phenomenon has the potential to develop into a strategy for controlling the thermomechanical energy of microporous liquids as well as for tuning the heat of wetting/dewetting of nanopores. This effective control would be relevant to a great variety of natural and technological processes such as the separation of liquids, liquid-phase chromatography, porosimetry, energy dissipation, conversion and storage,

biological and bioinspired channels and many more<sup>1</sup>. Particularly, we discuss these experimental and computational findings within the framework of the Horizon 2020 Electro-Intrusion<sup>2</sup> project dedicated to addressing these phenomena.

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1. Bartolomé, L. et al. Journal of Physical Chemistry Letters 15, 880-887 (2024).

2. ELECTRO INTRUSION Project. 2021. < https://www.electro-intrusion.eu/en >.

# Keywords

Intrusion-Extrusion

19

Liquids Metal organic frameworks Molecules

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# Full title of article

Tuning Wetting-Dewetting Thermomechanical Energy for Hydrophobic Nanopores via Preferential Intrusion

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# All authors

L. Bartolomé, A. Anagnostopoulos, A.R. Lowe, P. Ślęczkowski, E. Amayuelas, A. Le Donne, M. Wasiak, M. Chorążewski, S. Meloni, Y. Grosu

# DOI

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# P.056 Assessing nanoparticle coverage with biomimetic membranes via nanoplasmonics

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# Abstract

Despite their potential across a wide range of clinical applications, inorganic nanoparticles (NPs) suffer of limited biocompatibility and stability in biological fluids, which poses limitations to their clinical translation. To address these challenges, a common approach involves camouflaging the active inorganic core with a lipid bilayer coating, which provides biomimetic surface functions. While bilayer-coated NPs' design is rapidly advancing, achieving uniform membrane coverage and establishing efficient and accessible methods to quantify its integrity still represent major hurdles in the field.

In prior investigations, we demonstrated that the nanoplasmonics of AuNPs can sensitively probe key features of freestanding lipid bilayers (e.g., synthetic, and natural lipid vesicles), such as their concentration<sup>1</sup>, stiffness<sup>2</sup>, and protein inclusions<sup>3</sup>. Here, we extend this investigation to NPs-supported lipid bilayers, to evaluate the ability of AuNPs to assess bilayer coating integrity. bilayer on SiO<sub>2</sub>NPs drives AuNPs binding and spontaneous clustering, occurring at different extents depending on coating integrity<sup>4</sup>. Remarkably, we identified a linear relationship between membrane coverage and an optical descriptor of AuNPs' plasmonic properties, spanning over a wide range of coating yields<sup>4</sup>.

These findings offer a robust and cost-effective method to quantify the integrity of membrane coverage on NPs, crucial for a reliable assessment of new procedures for bilayer-coated NPs preparation and large-scale production. Furthermore, we introduce a straightforward and scalable procedure to prepare SiO<sub>2</sub>NPs/AuNPs hybrids with tuneable structural and plasmonic properties, templated by the lipid bilayer.



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[2] Nanoscale Horizons, 2021, 6, 543-550.

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[4] J. Colloid Interface Sci., 2023, 640, 100-109.

#### Keywords

membrane-coated nanoparticles nanoplasmonics biomimetic nanoparticles silica nanoparticles

#### Last published paper details

M. Puthia, J. Petrlova, G. Petruk, M. Butrym, F. Samsudin, M. Å Andersson, A.-C. Strömdahl, S. Wasserstrom, E. Hartman, S. Kjellström, L. Caselli, O. Klementieva, P. J. Bond, M. Malmsten, D. Bushan Raina, A. Schmidtchen. "Bioactive Suture with Added Innate Defense Functionality for the Reduction of Bacterial Infection and Inflammation (Adv. Healthcare Mater. 31/2023)." Advanced Healthcare Materials 12.31 (2023): 2370195.

#### Full title of article

Bioactive Suture with Added Innate Defense Functionality for the Reduction of Bacterial Infection and Inflammation

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# All authors

M. Puthia, J. Petrlova, G. Petruk, M. Butrym, F. Samsudin, M. Å Andersson, A.-C. Strömdahl, S. Wasserstrom, E. Hartman, S. Kjellström, L. Caselli, O. Klementieva, P. J. Bond, M. Malmsten, D. Bushan Raina, A. Schmidtchen

DOI

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# P.057 Novel fluorocarbon and hydrocarbon surfactants: Synthesis and comparative study of their behavior at the oil/water interface

<u>Syed Muhammad Shakil Hussain</u><sup>1</sup>, Muhammad Shahzad Kamal<sup>1</sup>, Shirish Patil<sup>1</sup>, Mohammed Alotaibi<sup>2</sup>, Mohanad Fahmi<sup>2</sup> <sup>1</sup>King Fahd University of Petroleum and Minerals (KFUPM), Saudi Arabia. <sup>2</sup>Saudi Aramco, Saudi Arabia

# Abstract

Enhanced oil recovery (EOR) techniques are used to produce the leftover oil after primary and secondary recovery. Using the EOR technique, around 60 % of the remaining crude oil can be recovered. Surfactant flooding is an industrially proven chemical-enhanced oil recovery (cEOR) technique that obtains trapped and residual oil by enhancing pore-scale displacement efficiency. However, the stability of surfactants at high temperatures and salinity reservoir environment and adsorption onto the reservoir rocks are the big issues these days.

Fluorocarbon and hydrocarbon surfactants were synthesized by adding a 1:2 ratio of suitable acid and amine followed by a quaternization reaction. The structure was differ only by fluorocarbon chain and hydrocarbon chain. The synthesized surfactants were confirmed by 1HNMR, 13CNMR, FT-IR, and mass tests to identify the chemical structure. The thermal stability was measured using Thermal Analysis (TGA) together with the aging technique. The surface/interfacial parameters were identified by force tensiometer and spinning drop method. The adsorption tests were conducted on dolomite and calcite using HPLC.

The synthesized surfactants displayed excellent solubility in normal and high salinity brine. The TGA graph exhibited that fluorocarbon surfactants are more thermally stable than hydrocarbon surfactants and the degradation temperature was above 250 °C which is higher than the reservoir

temperature ( $\geq 90^{\circ}$ C). Furthermore, the aging technique showed no cloudiness of the dissolved solution after putting them in an oven for up to 30 days at 90 °C. The surface analysis results were parallel to or greater than the commercial surfactants. The retention experiments showed that surfactant retention varies by varying rock samples due to the intercalation of surfactants with carbonates.

The results showed that the synthesized fluorocarbon and hydrocarbon surfactants exhibited high thermal stability, clear aqueous solutions, excellent surface parameters, and low adsorption onto carbonate rocks. All these parameters are important in cEOR and helpful in designing and developing material for enhanced oil production.

# Keywords

Surfactant Synthesis Surface Soft

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model fuels with sulfonated polystyrene as catalyst in ionic liquids. J Taiwan Inst Chem Eng 2020;115:128–34. https://doi.org/10.1016/j.jtice.2020.10.001. [8] Singh V, Amirchand KD, Gardas RL. Ionic liquid-nanoparticle based hybrid systems for energy conversion and energy storage applications. J Taiwan Inst Chem Eng 2022;133:104237. https://doi.org/10.1016/j.jtice.2022.104237.

# Full title of article

A review of ionic liquids: Recent synthetic advances and oilfield applications

# Journal

Journal of the Taiwan Institute of Chemical Engineers

# Year

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Background: lonic liquids have received a lot of interest in recent years from scientists and academics due to their distinctive qualities, including low vapor pressure, low toxicity, high thermal stability, and recyclability. Ionic liquids have become a more sustainable substitute for volatile organic solvents.

# All authors

Syed Muhammad Shakil Hussain,\* , Ahmad A. Adewunmi, Olalekan Saheed Alade, Mobeen Murtaza, Ahmad Mahboob, Hasan J Khan, Mohamed Mahmoud, Muhammad Shahzad Kamal

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# **P.058** Exploring novel approaches to develop an efficient lyophilization process for the stabilization of drug-loaded colloidal liposomes

<u>Akash Chaurasiya</u>, Kanan Panchal, Siddhant Padhi Birla Institute of Technology and Science, Pilani, Hyderabad Campus, India

#### Abstract

Liposomes are colloidal dispersion widely approved for drug delivery with better clinical performance. However, besides considerable advantages, their translation encounters challenges due to aqueous instabilities, leading to lipid/drug degradation, drug leakage, fusion/aggregation, etc. Usually, lyophilization technique is used to curb the unstable behaviour of this aqueous colloidal dispersion by forming a stable freeze-dried product. Although lyophilization is widely used, it is an extremely inefficient process with respect to high manufacturing costs and requires considerable time for product manufacturing and release. Thus, to overcome these challenges of lyophilizing a colloidal vesicular system, we have developed a robust, energy and time-efficient lyophilization process for the drug-loaded liposomes. To develop an efficient lyophilization process, various factors like selection of cryoprotectant, freezing rate, drying rate, etc., were identified and optimized. Drug-loaded liposomes were prepared using the standard thin film hydration method. Various cryoprotectants viz, mannitol, trehalose, sucrose, HPBCD, povidone K12 were assessed individually and in combination with liposomal preparations. These formulations were subjected to different processing conditions where the effect of normal freezing, annealing, faster drying, etc., were evaluated to obtain an efficient lyophilization process for liposomes. The resultant lyophilized products were then subjected to stability studies at real-time conditions (25°C/60%RH) and accelerated conditions (40°C/75%RH). The preliminary stability studies suggest stable behaviour of lyophilized liposomes using trehalose-HPBCD combination as cryoprotectants, with fast primary drying. During stability studies, no changes were observed in particle size, zeta potential, entrapment efficiency, drug assay, etc., of these lyophilized liposomes. These outcomes demonstrated a significant 3-fold reduction in lyophilization process duration, compared to the conventional process, without compromising the product attributes. The outcomes of this study using an optimum combination of cryoprotectants and a faster drying technique provide exciting results with possibilities of manufacturing lyophilized liposomes in an efficient, cost-effective and timely manner.

#### Keywords

Liposomes Colloidal dispersion Lyophilization Cryoprotectant

#### Last published paper details

Rani, Sarita, Sahoo Rakesh Kumar, Mahale Ashutosh, Panchal Kanan, Chaurasiya Akash, Kulkarni Onkar, Kuche Kaushik, Jain Sanyog, Nakhate Kartik Ajazuddin, Gupta Umesh, "Sialic Acid Engineered Prodrug Nanoparticles for Codelivery of Bortezomib and Selenium in Tumor Bearing Mice" Bioconjugate Chemistry, 2023, 34, 9, 1528–1552

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Sialic Acid Engineered Prodrug Nanoparticles for Codelivery of Bortezomib and Selenium in Tumor Bearing Mice

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#### All authors

Sarita Rani , Rakesh K Sahoo, Ashutosh Mahale, Kanan Panchal, Akash Chaurasiya, Onkar Kulkarni, Kaushik Kuche, Sanyog Jain, Kartik T. Nakhate, Ajazuddin, and Umesh Gupta

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# P.059 Hydroxypropyl beta-cyclodextrin coated paclitaxel nanocrystals: Safety and efficacy

Razan Haddad<sup>1</sup>, Nasr Alrabadi<sup>2</sup>, Bashar Altaani<sup>3</sup>, Majed Masadeh<sup>3</sup>, Tonglei Li<sup>4</sup>

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#### Abstract

**Background**: Paclitaxel (PTX) is one of the hydrophobic chemotherapeutic agents critical in the treatment of many cancers. Paclitaxel nanocrystals (PTX-NC), on the other hand, is a novel method for improving the delivery of paclitaxel by enhancing many properties such as its solubility and efficacy.

**Objectives**: Developing a novel PTX-NCs delivery system using the biocompatible/biodegradable hydroxypropyl-betacyclo-dextrin (HP $\beta$ CD) as a coating material aiming to improve its safety, efficacy, and targeting properties.

**Methods**: Here, PTX-NCs were prepared by the anti-solvent method followed by homogenization. Then, the surface of PTX-NC has been modified/coated using HP $\beta$ CD through the formation of a non-inclusion complex. The characteristics of this complex were approved in terms of size, polydispersity index, charge, morphology, crystallinity, release kinetics, and stability. Furthermore, the hemolytic assay and the cytotoxicity assays on both cancerous and normal cell lines were conducted to determine the safety, efficacy, and targeting properties of this coating modality.

**Results**: HP $\beta$ CD-PTX-NCs were relatively safe and are not expected to induce significant hemolytic activity after 1 and 3 hrs. of exposure compared to the control uncoated PTX-NCs. Moreover, significant growth inhibition was noticed for the HP $\beta$ CD-PTX-NCs on the MCF-7 cancer cells. On the other hand, both, the HP $\beta$ CD-PTX-NCs and the PTX-NCs can cause a significant but similar trend of growth inhibition or cytotoxicity on the MDA-MB-231 cancer cells after 12 and 24 hrs. of exposure. However, it showed a better and safer profile on the Vero C1008 normal cells compared to the uncoated NCs and the commercially available paclitaxel formula.

**Conclusion**: The results of this study emphasized that the prepared nano delivery system (HPβCD coated PTX-NCs) could be a promising candidate to enhance PTX efficacy and safety profile and to provide targeted PTX delivery to cancer cells.

#### Keywords

Coated nanocrystals Paclitaxel Surface modification HPβCD

#### Last published paper details

Alrabadi N, Hamdan M, Haddad R, Sabi SH, Masadeh MM, Alzoubi KH, Al-Batayneh KM. Development and Evaluation of the Efficacy and Toxicity of a New Hybrid Antimicrobial Peptide MY8. Curr Pharm Des. 2023;29(43):3488-3496. doi: 10.2174/0113816128277632231201043542. PMID: 38083884.

Development and Evaluation of the Efficacy and Toxicity of a New Hybrid Antimicrobial Peptide MY8

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Nasr Alrabadi, Maryam Hamdan, Razan Haddad, Salsabeel H Sabi, Majed M Masadeh, Karem H Alzoubi, Khalid M Al-Batayneh

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# P.060 Novel chitosan-based diclofenac nano-particles for sustained release delivery in liquid dosage form

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# Abstract

**Background**: The oral sustained-release dosage form is considered one of the most common and convenient delivery systems, especially for children. Biodegradable and biocompatible nanoparticles are considered powerful and useful tools that can be used for such purposes.

**Objectives and Methods**: Diclofenac was formulated to aim to delay drug release by its complexation with chitosan (16 or 30KD) followed by covering the complex with suitable fatty acid (oleic acid). Then the nanoparticles were dispersed in water using a suitable surfactant (Tween-20 or -80). The particle size was optimized to be less than 150nm. The following characteristics were studied as well: Drug Loading, polydispersity, surface charge, surface morphology, and *in-vitro* drug release. The pharmacokinetic characteristics were also studied in animals and humans.

**Results**: Sixteen different formulas were successfully prepared for diclofenac. All sixteen formulas were in the nanoparticle range (24.4-126 nm) and the drug loading efficiency was above 95%. The polydispersity index ranged from 0.246 to 0.62. Moreover, most of the particles appeared spherical under TEM microscopy and carried positive charges (up to 20.5 mv). Finally, the rate of drug release varies depending on the composition of the formulation; decreasing with the decrease of the ratio of chitosan, the decrease in its molecular weight, the increase of oleic acid, the use of Tween 20, and finally the decrease in surfactant ratio. Four formulas that release the drug for close to 24 hours were selected for the stability studies. All the formulations showed fair stability, however, the formula with 16KD-chitosan and Tween-80 showed a superior long-term stability profile. The latest formula showed promising pharmacokinetic profiles in dogs and humans compared to the commercially available diclofenac tablets.

**Conclusions:** The novel chitosan-based nanoparticles can be a promising liquid delivery tool for diclofenac and other NSAIDs, especially for children.

# Keywords

Nano-particles Chitosan Diclofenac Sustained Release Delivery

#### Last published paper details

Alrabadi N, Hamdan M, Haddad R, Sabi SH, Masadeh MM, Alzoubi KH, Al-Batayneh KM. Development and Evaluation of the Efficacy and Toxicity of a New Hybrid Antimicrobial Peptide MY8. Curr Pharm Des. 2023;29(43):3488-3496. doi: 10.2174/0113816128277632231201043542. PMID: 38083884.

# Full title of article

Development and Evaluation of the Efficacy and Toxicity of a New Hybrid Antimicrobial Peptide MY8

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# All authors

Nasr Alrabadi\*, Maryam Hamdan, Razan Haddad, Salsabeel H. Sabi, Majed M. Masadeh, Karem H. Alzoubi, Khalid M. Al-Batayneh

# DOI

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# **P.061** Interactions of gadolinium with brain membranes are defined by the headgroup structure and acyl chain architecture of key lipids

Kianmehr Farzi<sup>1</sup>, <u>Travis Issler</u><sup>1</sup>, Colin Unruh<sup>2</sup>, Elmar Prenner<sup>1</sup> <sup>1</sup>University of Calgary, Canada. <sup>2</sup>Fuel Innovation Calgary, Canada

# Abstract

Biological membranes are key components of all cellular systems that provide the structural integrity for cells and organelles, but are also key sites of signalling. Inherently, membranes are the first point of interaction between cells, and both biologically relevant as well as toxic exogenous materials. The latter includes metal pollutants that have progressively increased due to anthropogenic activity, leading to public health concerns. Metals are used in many industries. The lanthanide metal, gadolinium (Gd), has been applied in the health sciences as a contrast agent in complex with different chelates (gadolinium-based contrast agent, GBCA) during magnetic resonance imaging (MRI). It has been shown that GBCA administration may lead to Gd deposition in both the brain and kidneys of patients. The potential deposition in the brain motivated this study to focus on the impact of Gd at the level of the cell membrane.

Biophysical analyses of membranes comprised of sphingomyelins, phosphatidylcholines, and brain polar lipid extracts were investigated by fluorescence spectroscopy and dynamic light scattering to assess metal effects on membrane fluidity and liposome size. The results demonstrate that the effects of Gd depend on the detailed lipid architecture and the lipid composition of membranes. Lipids with saturated acyl chains exhibit stronger changes in the presence of Gd. As seen for other cations, Gd has strong interactions with anionic lipids, presumably due to electrostatic interactions, leading to increases in membrane rigidity and liposome size. In addition, Gd also showed strong effects on zwitterionic lipids, phosphatidylcholines and especially sphingomyelins. Furthermore, Gd effects at low micromolar concentrations are comparable to effects of metals such as cadmium and lead but at concentrations an order of magnitude higher. These observed effects, especially on sphingomyelins, a key brain lipid class, are concerning and require more research.

#### Keywords

Gadolinium Membrane Rigidity Brain Lipids Sphingomyelin

# Last published paper details

Farzi, K.; Issler, T.; Unruh, C.; Prenner, E.J. Gadolinium Effects on Liposome Fluidity and Size Depend on the Headgroup and Side Chain Structure of Key Mammalian Brain Lipids. Molecules 2024, 29, 135. https://doi.org/10.3390/molecules29010135

#### Full title of article

Gadolinium Effects on Liposome Fluidity and Size Depend on the Headgroup and Side Chain Structure of Key Mammalian Brain Lipids

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Farzi, K.; Issler, T.; Unruh, C.; Prenner E.J

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# P.062 Molecular aggregation strategy for inhibiting DNases

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#### Abstract

This research uncovers the unique capability of molecular aggregation to inhibit a protein linked to disease. Enzyme inhibitors, often developed as targeted drugs, have been utilized in treating cancer, autoimmune diseases, and infections.

needing bivalent metal ions. A DNase released by Streptococcus pyogenes triggers streptococcal toxic shock syndrome (STSS), a critical infectious disease with over 30% mortality rate even today. S. pyogenes compromises the human defense against infections via DNase secreted by them. Developing an inhibitor for this DNase has been a significant challenge. Our findings show that Mn007 aggregates can inhibit this DNase from S. pyogenes, effectively curbing the growth of the bacteria in human blood. This study indicates that molecular aggregation, previously overlooked in drug development, represents an untapped potential in the field. It demonstrates that small molecule compounds, through aggregation, can effectively inhibit enzymes associated with diseases, opening new avenues in drug discovery and development.

# Keywords

deoxyribonuclease inhibitor aggregation streptococcus pyogenes

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# P.063 Highly conductive riboflavin-based carbon quantum dot–embedded SiO<sub>2</sub>@MoS<sub>2</sub> nanocomposite for enhancing bioelectricity generation through synergistic direct and indirect electron transport

<u>Yi-Ho Kuo</u> Kaohsiung Medical University, Taiwan

# Abstract

A microbial fuel cell (MFC) is an advanced green battery that has limited application because of its low current density. In the present study, *Shewanella oneidensis* MR-1, which is an electricity-producing bacterium, was used in an electrochemical reactor as a bacterial model. Mesoporous spherical silica nanoparticles (NPs) loaded with riboflavin (RF) were prepared as the starting material, following which surface modification was conducted to

expose the thiol group, which considerably increased the affinity of the NPs to  $MoS_2$  and resulted in the formation of a dense  $MoS_2$  shell on the surface after calcination. Moreover, the loaded RFs were successfully transformed into RF-based carbon quantum dots (CQDs), which resulted in a substantial increase in conductivity. The CQD-embedded  $SiO_2@MoS_2 NPs$ , which contained redox-active N-doped CQDs and had a metallic  $MoS_2$  shell, were able to receive electrons from exoelectrogenic bacteria (charging) and transfer electrons to an indium tin oxide electrode (discharging). Thus, these NPs could act as an electron nanoshuttle and a conductive medium in biofilms for enhancing systematic extracellular electron transport. A 10-fold increase in bioelectricity production than no NPs addition was achieved, which confirmed the applicability of the aforementioned NPs in advanced MFC applications. The NPs prepared in this study, which mimic biological electron shuttles (e.g., RF) in long-distance conduction, can usher in a new era in the development of advanced MFCs.

# Keywords

microbial fuel cell molybdenum disulfide carbon quantum dot extracellular electron transport

# Last published paper details

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# Full title of article

Highly conductive riboflavin-based carbon quantum dot-embedded SiO2@MoS2 nanocomposite for enhancing bioelectricity generation through synergistic direct and indirect electron transport

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# All authors

Yi-Ho Kuo, Ming-Chien Hsu, Wen-Jyun Wang, Hung-Hsi Peng, and Wei-Peng Li\*

# DOI

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# P.064 Photo-responsive ascorbic acid-modified Ag<sub>2S</sub>–ZnS heteronanostructure dropping pH to trigger synergistic antibacterial and bohr effects for accelerating infected wound healing

Kaohsiung medical university, Taiwan

# Abstract

Nonantibiotic approaches must be developed to kill pathogenic bacteria and ensure that clinicians have a means to treat wounds that are infected by multidrug-resistant bacteria. This study prepared matchstick-like Ag2S-ZnS heteronanostructures (HNSs). Their hydrophobic surfactants were then replaced with hydrophilic poly(ethylene glycol) (PEG) and thioglycolic acid (TGA) through the ligand exchange method, and this was followed by ascorbic acid (AA) conjugation with TGA through esterification, yielding well-dispersed PEGylated Ag2S-ZnS@TGA-AA HNSs. The ZnS component of the HNSs has innate semiconductivity, enabling the generation of electron-hole pairs upon irradiation with a light of wavelength 320 nm. These separate charges can react with oxygen and water around the HNSs to produce reactive oxygen species. Moreover, some holes can oxidize the surface-grafted AA to produce protons, decreasing the local pH and resulting in the corrosion of Ag<sub>2</sub>S, which releases silver ions. In evaluation tests, the PEGylated Ag<sub>2</sub>S–ZnS@TGA-AA had synergistic antibacterial ability and inhibited Gram-negative Escherichia coli and Gram-positive methicillinresistant Staphylococcus aureus (MRSA). Additionally, MRSA-infected wounds treated with a single dose of PEGylated Ag<sub>2</sub>S–ZnS@TGA-AA HNSs under light exposure healed significantly more quickly than those not treated, a result attributable to the HNSs' excellent antibacterial and Bohr effects.

# Keywords

methicillin-resistant Staphylococcus aureus Heteronanostructure Bohr effect wound healing

# Last published paper details

ACS Applied Materials & Interfaces, 2024, 16, 12018–12032.

# Full title of article

Photo-Responsive Ascorbic Acid-Modified Ag2S–ZnS Heteronanostructure Dropping pH to Trigger Synergistic Antibacterial and Bohr Effects for Accelerating Infected Wound Healing

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# All authors

Li-Ting Yang, Wen-Jyun Wang, Wan-Ting Huang, Liu-Chun Wang, Ming-Chien Hsu, Chung-Dann Kan, Chun-Yung Huang, Tak-Wah Wong, and Wei-Peng Li

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# P.065 Generation of ferrofluid microdroplet or micro-hydrogels in microfluidic cross-junction microchannel with a shrinking nozzle

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<sup>1</sup>Southern University of Science and Technology, China. <sup>2</sup>Doshisha University, Japan

# Abstract

Microdroplet generated in microfluidic chip has been great potential on chemistry and medicine. However, the underlying fluid mechanisms are still not well understood. Exploring the flow behavior and interface deformation can provide a precise controlling method for the droplet generation. To achieve that, a Polydimethylsiloxane (PDMS) based microfluidic cross-junction microchannel with a shrinking nozzle, and a magnetic field coupling multiphase lattice Boltzmann method are developed for the experimental and numerical investigations, respectively. The shearing process and the interface deformation of ferrofluid are controlled by microfluidic pump and observed through the microscopy and high-speed camera. Both experimental and numerical results demonstrate that the shrinking nozzle structure has a positive impact on the reducing the droplet size. For the generation of magnetic micro-hydrogels, the magnetic nanoparticles are first synthesized by chemical coprecipitation method, and then coated with surfactant. The compound aqueous ferrofluidic cross-junction microchannel to generated magnetic microdroplets. These microdroplets are immediately transferred into a calcium chloride solution which is used as cross-linking agent in present work. Finally, the isotropic, monodispersed, and biocompatible magnetic micro-hydrogels can be obtained.

# Keywords

Ferrofluids magnetic micro-hydrogels lattice Boltzmann method microfluidic chips

# Last published paper details

X. Li, Z.Q. Dong, Y. Y. Li, H. Yamaguchi, and P. Yu\*, "Magnetic field induced acceleration or deceleration of bubble rising inside ferrofluids: a fractional step lattice Boltzmann investigation," J. Magn. Magn. Mater., 591, 171750 (2024).

# Full title of article

Magnetic field induced acceleration or deceleration of bubble rising inside ferrofluids: a fractional step lattice Boltzmann investigation

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# **P.066** The magnetic self-assembly of non-magnetic particles in ferrofluids and its application on anisotropic thermal conductivity CNT/PDMS composite

# Zhi-Qiang Dong<sup>1</sup>, Xiang Li<sup>1</sup>, Hiroshi Yamaguchi<sup>2</sup>, Peng Yu<sup>1</sup>

<sup>1</sup>Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology, China. <sup>2</sup>Energy Conversion Research Center, Doshisha University, Japan

# Abstract

In the present study, the magnetic field induced self-assembly processes of non-magnetic microparticles dispersed in aqueous ferrofluids are experimentally and numerically investigated. The non-magnetic microparticles are formed into the chain-like microstructures when applying an external uniform magnetic field. The length of these self-assembled chain-like microstructures are measured in a microfluidic chip. Further, a three-dimensional (3D) numerical model based on multiple-relaxation-time lattice Boltzmann method (MRT-LBM) is developed to simulate the self-assembly process of non-magnetic microparticles in a microchannel. The chain-like microstructures under different magnetic intensities are calculated, and their distribution and the average length are investigated. The coincident results of the experiments and numerical simulations provide a guidance on non-contact manipulate the non-magnetic materials to form the chain-like structures by magnetic field. Finally, the anisotropic thermal conductivity composite materials are obtained by first dispersing the carbon nanotube (CNT), magnetic nanoparticles with surface modification and the cross-linking agent into Polydimethylsiloxane (PDMS) base, and then applying a uniform magnetic field during the curing process of PDMS. The thermal conductivity along and perpendicular to the magnetic field are measured, respectively. Besides, compared with the disordered structures inside CNT/PDMS composite without magnetic effect, the ordered self-assembled CNT structures can provide an anisotropic property. This work demonstrates the great potential of magnetic self-assembly of nonmagnetic materials in ferrofluids on manufacturing the functional materials.

# Keywords

self-assembly ferrofluids functional composite lattice Boltzmann method

#### Last published paper details

Z.Q. Dong, X. Li, H. Yamaguchi, and P. Yu\*, "Magnetic field effect on the sedimentation process of two non-magnetic particles inside a ferrofluid," J. Magn. Magn. Mater., 589, 171501 (2024).

#### Full title of article

Magnetic field effect on the sedimentation process of two non-magnetic particles inside a ferrofluid

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# P.067 Effects of intentionally introduced defects on the mechanical, chemical, and structural properties of metal oxide nanostructures

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# Abstract

This study investigates the impact of intentionally introduced defects on the mechanical, chemical, and structural properties of metal oxide nanostructures. Through controlled defect formation on the surfaces of these nanostructures, we explore the resulting modifications in their behavior. The mechanical responses, chemical reactivity, and overall structural characteristics are analyzed to provide insights into the influence of defects on these crucial aspects. This research contributes to a deeper understanding of the tailored manipulation of metal oxide nanostructures for various applications, spanning from catalysis to advanced materials engineering.

To gain insights into the optimized surfaces of metal oxides and their chemical composition, we conducted thorough surface analyses using advanced techniques such as X-ray Photoelectron Spectroscopy (XPS) and Transmission Electron Microscopy (TEM). Furthermore, we conducted a comprehensive investigation to determine the optimal operating temperature and selectivity of the materials.

Furthermore, the metal oxide nanoparticles with surface modifications presented in this study exhibit considerable potential for practical applications across various domains. The improved properties and optimized performance characteristics render them highly valuable for incorporation into next-generation electronic components, holding promise for the advancement of electronic technologies. The outcomes of this research create novel possibilities for leveraging the advantages of surface-modified metal oxide nanoparticles, thereby contributing to the ongoing progress in electronic materials and devices.

# Keywords

Surface modification defect vacancy activity

# Last published paper details

Two-Dimensional calcium silicate nanosheets for trapping atmospheric water molecules in humidity-immune gas sensors

# Full title of article

Two-Dimensional calcium silicate nanosheets for trapping atmospheric water molecules in humidity-immune gas sensors

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# All authors

Young Ju Cho, Yong Jung Kwon, Sunghwan Jin, Hyeunseok Choi, Jung-Hoon Lee, Seung-Min Yang, Sun-Woo Choi, Young Kyu Jeong

# DOI

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# **P.068** Improving flotation of fine valuable lithium minerals through the formation of small hydrophobic flocs

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<sup>1</sup>University of Melbourne, Australia. <sup>2</sup>Future Battery Industries Cooperative Research Centre, Australia. <sup>3</sup>ARC COE for Enabling Eco-efficient Beneficiation of Minerals, Australia

# Abstract

The escalating demand for lithium, primarily driven by the rapid development of electronic devices and new energy vehicles, necessitates the efficient recovery of lithium from spodumene, its main industrial source. The commonly employed method of flotation, however, poses significant challenges when recovering fine spodumene particles due to inefficient bubble-particle attachment. The present study investigates an innovative approach to improve the flotation efficiency of these fine particles through selective flocculation. We aim to aggregate fine spodumene particles to a size (~100 µm) using commercially available flocculants to enable efficient recovery in froth flotation. A crucial aspect of our research focuses on the selective flocculation of spodumene from other gangue minerals like feldspar and quartz using commercial polymers. The aggregate size is measured in-situ using a particle imaging and sizing probe under shear conditions expected in mechanical flotation cells. The study also delves into the use of metal ions as activators, a technique adapted from their recognized ability to enhance the adsorption of fatty acid collectors during flotation. Further investigation on the optimum collector reagent will be conducted. The promising findings if implemented could significantly improve the recovery of fine spodumene that currently goes to tailings. This technology could help satisfy the growing global lithium demand.

# Keywords

Polymeric Selectivity in Mineral Processing Lithium Recovery Fatty Acid Collectors Sustainable Mining Practices

## Last published paper details

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# P.069 Improving the collection of fine copper minerals via aggregation using polyacrylamide polymers

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# Abstract

Copper is one of the key elements for a low-carbon future and a global transition into renewable energy, being fundamental for the construction of solar cells, electric vehicles, wind turbines, and energy storage devices. Nowadays, copper minerals such as chalcopyrite are industrially separated from other waste minerals (e.g. guartz) through flotation processes, where the materials are separated based on their hydrophobicity differences. In this process, the valuable mineral is made hydrophobic and rises to the top of the flotation cell, where it is collected. However, industrial flotation has been limited to collecting particles ranging between 50-150 µm sizes, which results in significant losses of valuables below and above that size. The present work aims to use the flocculation-flotation approach to improve the recovery of fine copper minerals. In this approach, commercial polyacrylamide polymers were used to selectively increase the size of fine valuable minerals via flocculation, to produce aggregates that are in the suitable size for froth flotation. The effect of the polymer characteristics such as charge and molecular weight, as well as the shear input in the cell, was investigated on the aggregate sizing and formation. The results indicated that both cationic (CPAM) and anionic (APAM) polymers can effectively aggregate chalcopyrite, however, the cationic polymer is not selective towards the target valuables, as it also aggregates quartz. Furthermore, it was observed that the flocculant's molecular weight and shear intensity also have an important influence on the flocculation performance, with higher MW polymers and lower shear inputs producing bigger and stronger aggregates, that are more likely to survive the flotation cell.

# Keywords

Particle aggregation In-situ image characterization Polymer adsorption Sizing analysis

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# P.070 Synthesis of Ni-Fe layered double hydroxide through continuous flow process for oxygen evolution reaction

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## Abstract

The necessity for highly efficient, noble metal-free oxygen evolution reaction (OER) electrocatalysts is driven by the sluggish kinetics of OER, leading to reduced efficiency in water splitting electrochemical cells. Transitionmetal layered double hydroxide (LDH) materials are emerging as potent OER electrocatalysts, rivaling traditional noble-metal oxides like IrO<sub>2</sub> and RuO<sub>2</sub>. Conventionally, LDHs are produced *via* a batch co-precipitation method, which, however, restricts their scalability for industrial use. This research introduces a novel approach for the mass production of Ni-Fe LDHs using a continuous flow synthesis method. The process involves a continuous stirred tank reactor where metal and base precursor solutions are injected concurrently. The synthesized Ni-Fe LDHs are analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS) under various conditions like reaction temperature, time, and solution concentrations. The electrochemical catalytic efficiency of Ni-Fe LDHs for OER is similar to that of LDHs produced by a batch co-precipitation, which indicates successful continuous flow synthesis of Ni-Fe LDHs on a large scale.

# Keywords

oxygen evolution reaction layered double hydroxide continuous flow process co-precipitation

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## All authors

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# P.071 Hyaluronic acid/pectin immune active nanogels formed via photocrosslinking for transcutaneous delivery

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## Abstract

Nanogel is a promising drug carrier for both topical and systemic deliveries. Particularly recent studies have highlighted that nanogels can be delivered by penetrating the stratum corneum. The aim of this study is to fabricate nanogels with hyaluronic acid/pectin and evaluate their immune activity to antigen presenting cells. For photocrosslinking, both pectin that was isolated from *Ulmus davidiana* var. *japonica* (Rehder) Nakai (Japanese elm) (UDP) and hyaluronic acid (HA) were modified with methacrylic anhydride. Nano-sized particles were formed by water-in-oil emulsification with the prepolymer solution (discontinuous phase) and surfactant-dissolved hexane (continuous phase). Then crosslinking was conducted via a brief UV light curing. The resulting nanogels' size was in the range of 100–300 nm in diameter and skin penetration test using porcine skin revealed that the hybrid HA-UDP nanogels were deposited in the epidermis as well as the dermis by penetrating the stratum corneum. In the case of cellular response, upregulation of multiple inflammatory cytokines was observed in macrophages that internalized HA-UDP nanogels. This indicates that the hyaluronic acid/pectin hybrid nanogels can be used as an immunomodulator for treatment of skin irritation and inflammation.

## Keywords

Nanogel Hyaluronic Acid Pectin Transcutaneous drug delivery

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# P.072 The role of Ni doping on thermoelectric performance of n-type Bi1.8-xSb0.2Te3 system

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# Abstract

This research paper presents a comprehensive investigation into the structural and thermoelectric properties of Ni-doped  $Bi_{1.8-x}Ni_xSb_{0.2}Te_3$  (x =0, 0.02, 0.04, 0.06, 0.08) samples synthesized using a fast and cost-efficient conventional solid-state reaction technique. X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses confirm the absence of any impurities in the synthesized samples. The crystal structure of the prepared samples belongs to the RM space group, exhibiting a rhombohedral crystal structure. The synthesized samples demonstrate n-type behaviour, with a carrier concentration of the order of 10<sup>19</sup>/cm<sup>3</sup> and samples shows the degenerate semiconducting behaviour. A detailed comparison with pristine samples reveals a noteworthy enhancement in conductivity at room temperature, particularly evident for the Ni doping level of x = 0.04. The room temperature conductivity increases from 60 S/cm to 120 S/cm, due to the enhanced carrier mobility resulting from Ni doping at the Bi sites. Furthermore, increase in carrier concentration, in turn, elevates the power factor of the material. Notably, the promising thermoelectric properties observed, especially near room temperature, underscore the potential of Ni-doped Bi<sub>1.8-x</sub>Ni<sub>x</sub>Sb<sub>0.2</sub>Te<sub>3</sub> as effective materials for thermoelectric applications. This research contributes valuable insights into the optimization of thermoelectric materials through controlled doping strategies, opening avenues for the development of efficient and economically viable thermoelectric devices.

# Keywords

Thermoelectrics Doping Thermal conductivity carrier concentartion

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## Full title of article

Influence of microstructure and thermoelectric properties on the power density of multi-walled carbon nanotube/ metal oxide hybrid flexible thermoelectric generators

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## All authors

Ramakrishna Nayak , Prakasha Shetty , M. Selvakumar , B. Shivamurthy , Ashok Rao , K.V. Sriram , M.S. Murari , Akshayakumar Kompa , U. Deepika Shanubhogue

# P.073 Rheological study on surfactant packages and polymers for chemical enhanced oil recovery

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## Abstract

The application of surfactants and polymers together is common in chemical enhanced oil recovery to enhance crude oil production. Polymers modify the flow properties, and increase the viscosity of brine. These polymers possess viscoelastic properties of polymer solution, aiding in achieving the desired viscosity increase and allowing them to pass through the porous medium without a critical pressure increase. The applied surfactants can interact with the polymers, making it important to jointly study these surfactant-polymer systems, including rheological properties, viscosity curves, and determination of loss and storage modulus. In our work the rheological properties of various polymer-surfactant combinations and drew conclusions about their interactions and applicability were systematically examined.

## Keywords

chemical enhanced oil recovery flow modifier polymer surfactants rheological properties

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Relationship between Some Colloidal Properties of Non-Ionic-Anionic Surfactant Mixtures

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# All authors

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# DOI

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# P.074 Development of determination method for the water number of surfactants

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## Abstract

The water number can be determined most simply by the conventional titration method. This procedure is a quick and reliable analytical method that helps understand the main properties of the tested surfactant. Although a well-established method for determining the water number has long been available, it has been revealed that the auxiliary substances used in this process are severely harmful to health, leading to the discontinuation of routine laboratory application. Therefore, it is crucial to review and improve the method.

Our aim was to replace the solvent mixture employed in the method with a mixture that has suitable properties for the water number determination method, while also posing minimal occupational safety risks. It is also expected to be less harmful than the currently used solvent and easily and cost-effectively obtainable.

## Keywords

Surfactants HLB Water number Method development

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# P.075 Fingering instability during the dewetting of nanocapillary suspensions

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# Abstract

Capillary suspensions are created by adding a small amount of immiscible secondary fluid to a conventional suspension, thus forming a sample-spanning network between the microparticles and significantly influencing the rheological behavior [1]. Although incorporating nanoparticles inside the liquid bridges enhances the compressive strength in sintered porous materials [2], they have been shown to weaken the network structure in the precursor suspension and enhance inter-microparticle movement [3].

In this study, the dewetting dynamics of capillary (nano)suspensions are investigated in a lifted Hele-Shaw cell using two synchronized high-speed video systems. The cell consists of two parallel solid plates (initial gap 50  $\mu$ m), one of which is lifted with a constant acceleration (up to 180 m/s<sup>2</sup>). The microparticles are fluorescently dyed for particle tracking. The dewetting of the liquid bridge is accompanied by the appearance of fingers, formed due to the Saffman-Taylor instability. The patterns are analyzed using machine learning-based image processing algorithms to extract the number of fingers and total dendritic area. The main parameters of the fingering patterns are compared for suspension combinations with and without microparticles, secondary fluid, and nanoparticles. We observed an increase in the number of fingers and the total dendritic area when particles are added to a pure liquid, but a decrease when a secondary fluid is added to the suspension due to the strong particle network. However, when nanoparticles are added, despite the weakened rheological response of the bridges, the fingering is further suppressed. Our findings provide new insights into the interplay between micro- and nanoparticle properties, capillary bridges, and flow instabilities in confined geometries with potential applications in microfluidics, 3D printing, and thin-film coatings.

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# Keywords

Capillary suspension Fingering instability Liquid bridge Interfacial tension

Last published paper details

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## Full title of article

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# All authors

YT Aksoy, L Liu, M Abboud, MR Vetrano, E Koos

# DOI

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# P.076 Investigating volume phase transition in electrostatics-driven supracolloidal gels

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# Abstract

Supracolloidal gels are three-dimensional fractal networks composed of transiently assembled colloids in dispersion. They form when attractive interactions between individual colloids are sufficiently high to overcome repulsion and thermal energy but, simultaneously, low enough to avoid precipitation. Although supracolloidal gels are already used for haptics customization in food and cosmetics, they are considered auspicious candidates for biocompatible inks in 3D printing and biomimetic scaffolds for cell encapsulation. [1] Thermoresponsive microgels are interesting model systems to examine the formation of physical supracolloidal gels as the interparticle interactions change with the volume phase transition from soft to hard colloid. [2] In electrostatics-driven supracolloidal gels, however, the extent to which colloidal softness and volume phase transition influence the mechanical properties and architecture of the gels is still unknown.

Herein, we present the complex temperature dependence of supracolloidal gels whose attractive forces originate in the electrostatic attraction of oppositely charged, thermoresponsive microgels. We prepared weakly acidic and weakly basic poly(*N*-isopropylacrylamide)-based microgels of the same size and verified the integration of the respective comonomer by FTIR or <sup>1</sup>H-NMR spectroscopy and electrophoretic mobility. When mixing oppositely charged microgels, supracolloidal gels form well below volume fractions necessary for colloidal glass transition, and electrostatics-driven gelation can be differentiated from hydrophobic crowding mechanisms. While the elasticity of electrostatics-driven supracolloidal gels depends on the temperature, the relation between storage modulus and temperature changes when the microgels overcome their volume phase transition temperature. Comparing the results from rheology to scattering and microscopy data allows deductions regarding the behaviour of individual microgels within the supracolloidal gel.

S. M. Morozova et al., ACS Nano 17 (2023) 15012–15024.
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## Keywords

supracolloidal gel thermoresponsive microgel electrostatic interaction self-assembly

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# P.077 Innovative crosslinking strategies in stimuli-responsive microgels: Beyond covalent bonds

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## Abstract

Stimuli-responsive microgels consist of colloidal polymer networks that are typically crosslinked via covalent bonds. However, the properties of those microgels such as their mechanical softness or degradation potential are significantly influenced by the specific nature of crosslinking within the polymeric network. As alternative for covalent crosslinks, supramolecular, hydrophobic, or electrostatic interactions can be used. [1] Among the non-covalent interactions,  $\pi$ - $\pi$  stacking enables the formation of highly stable, self-assembled structures.

In our synthesis approach, we explore aromatic peptide and liquid crystalline motifs for noncovalent crosslinking, as those material classes are known for their ability to self-organize into well-defined supramolecular architectures. The short aromatic peptide derivative diphenylalanine, bearing the Phe-Phe motif, has been utilized as a highly versatile selfassembling building block in nanotechnologies, whereas liquid crystals are known for exhibiting self-organization in response to external stimuli, such as changes in temperature. [2]

In this work, we study the synthesis and properties of temperature-responsive poly-*N*-vinylcapolactam-based microgels prepared by precipitation polymerization. Instead of covalent crosslinking,  $\pi$ - $\pi$  stacking interaction of co-monomers induces the crosslinking of polymer chains. Firstly, the compounds containing either the Phe-Phe motif or a liquid crystalline moiety were functionalized with a polymerizable acrylate group. The co-monomer content of the microgels was studied by Raman spectroscopy and <sup>1</sup>H-NMR. The morphology of the microgels was investigated by electron microscopy and dynamic light scattering. Further, we explored the degradation of microgels through ultrasonication or organic solvents, which has the potential for controlled release and delivery of biomacromolecules. [3]

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# Keywords

thermoresponsive microgels supramolecular interactions self-assembly precipitation polymerization

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## Full title of article

Kinetic Modeling of a Poly(N-vinylcaprolactam-co-glycidyl methacrylate) Microgel Synthesis: A Hybrid In Silico and Experimental Approach

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# P.078 Coarse-grained ssDNA with dissipative particle dynamics

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# Abstract

Dissipative Particle Dynamics (DPD) is a mesoscale tool bridging the gap between microscopic atomistic simulation and macroscopic thermophysical modelling. DPD has become highly popular for studying self-assembling polymer and surfactant solutions where the interactions can be mapped to the Flory-Huggins parameters<sup>1</sup>. However, only a few articles have tried to model the behaviour of single-stranded DNA (ssDNA). One such article by Valdivia et al.<sup>2</sup> simulated a Single-walled carbon nanotube (SWCNT) transmembrane channel formation in a pure 1,2-dimyristoylsn-glycero-3-phosphorylcholine (DPMC) bilayer with ssDNA using a combination of computational techniques: DPD-Monte Carlo hybrid simulations and quantum mechanical calculations at a hybrid-DFT level. In our work, we employ the same model as Valdivia et al.<sup>2</sup> to validate the transferability of the model parameters. The ssDNA model comprises a 25-nucleotide chain with hydrophilic and hydrophobic segments representing phosphate/pentose and nucleic acid bases, respectively; see the figure below for more details. We aim to evaluate the DPD model's effectiveness in capturing ssDNA-water equilibrium behaviour and dynamics, compare it with experimental results, and enhance our understanding of these complex mesoscale systems.



This study used a coarse-grained model for single-stranded DNA (ssDNA). Beads were represented by letter symbols and color-coded in simulation snapshots: A (purple), C (pink), G (yellow), T (lime), Pentose (orange), and Phosphate (grey).



coarse-grained model for ssDNA (25 nucleotides) used in this study

Soft repulsion parameters a<sub>ii</sub> used in this study for a system composed of one ssDNA chain.

1	1	ŋ	5	J 1		
a <sub>ij</sub>	W	H*	Α	С	G	Т
Ŵ	25					
Н	15	35				
Α	65	75	25			
С	55	65	35	25		
G	52	62	38	28	25	
Т	62	72	28	32	35	25

H\*: It represents pentoses and phosphates, i.e., the hydrophilic backbone, which was treated as head group beads "H" for simplicity.

# **DPD** Simulations



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## Keywords

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## Full title of article

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# All authors

Esam Hamid Hummadi, Yarkin Cetin, Merve Demirbek, Nadeems M. Kardar, Shazia Khan, Christopher J. Coates, Daniel C. Eastwood, Ed Dudley, Thierry Maffeis, Joel Loveridge and Tariq M. Butt

# DOI

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# P.079 Sorbents and biosorbents for the removal of the persistent pollutant ofloxacin

Filomena Sannino<sup>1</sup>, Alessandro Latte<sup>2</sup>, Zohreh Saedi<sup>2</sup>, Abu Yousuf<sup>3</sup>, Moreno Rizzo<sup>2</sup>, <u>Domenico Pirozzi</u><sup>2</sup> <sup>1</sup>Department of Agricultural Sciences, University of Naples "Federico II", Portici (NA), Italy. <sup>2</sup>Department of Chemical Engineering, Materials and Industrial Production (DICMaPI), University "Federico II", Naples,, Italy. <sup>3</sup>Department of Aerospace and Mechanical Engineeering, University of Oklahoma, Norman (Ok), USA

# Abstract

Ofloxacin (OFL) is a fluoroquinolone antibiotic used to treat many bacterial infections. It is particularly effective against Gram-negative bacteria and most enterobacteria, as it is able to inhibit the synthesis of bacterial nucleic acid [1]. Unfortunately, the degradation of this antibiotic due to human metabolism is incomplete (about 10%), and consequently large amounts of OFL, eliminated by urinary excretion, are contained in both the hospital and municipal wastes [2]. In addition, the industrial production of OFL contributes to release this antibiotic into wastewaters.

OFL is considered a particularly harmful persistent drug, as it cannot be completely removed in wastewater treatment plants, and consequently the effluents of these plants can contaminate surface waters, groundwaters and sediments. The OFL may bring, even at low concentrations, a strong ecological threat to cyanobacteria and aquatic plants. In addition, it can promote bacterial resistance through induction and selection, thus reducing the human ability to fight bacterial strains [3].

In this study, three different adsorbents are tested to develop an efficient OFL removal process:

1.chitosan hydrogels are bioavailable, ecologically sustainable materials, already tested in the removal of different classes of pollutants;

2.cyclodextrin nanosponges, natural oligosaccharides showing a hydrophilic external surface, responsible for hydrosolubility, and a hydrophobic inner cavity, allowing the incapsulation of a wide range of molecules;

3. *Arthrospira platensis* (Spirulina), a blue-green alga already used for the biosorption of many pollutants.

For each adsorption system, the selectivity towards OFL removal was studied. In addition, potential protocols for the desorption and the reuse of the adsorbent were explored. The influence of simultaneous adsorption of different drugs and ions was also investigated.

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- [3] Nguyen et al. (2021). Environmental Pollution, 291, 118095.

## Keywords

ofloxacin chitosan nanosponge Spirulina

## Last published paper details

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D. Pirozzi, A. Latte, F. Sannino

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# P.080 3D-printed porous polyamide-Li2TiO3 composite for efficient recovery of lithium

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# Abstract

Lithium has been included in the list of critical raw materials in Europe. Considering its current demand for LIBs production, lithium recycling technologies are in high urgency. Adsorption method has a great potential to be applied for lithium separation due to simplicity and low operational costs. However, adsorbent materials usually are powders that complicates their regeneration and reuse. Embedding of powders with formation of pellets, granules, foams, etc. causes the coverage of adsorption sites by the binder and decreased adsorption performance. In the current work additive manufacturing technology was applied for preparation of 3D-printed composite materials for selective adsorption of lithium ion from water. Polyamide powder PA2200 was used as support material. Active material was commercial Li<sub>2</sub>TiO<sub>3</sub> powder. Selective laser sintering method was

used for 3D-printing of monolith adsorbents. The surface morphology was examined with SEM equipped with EDS for elemental analysis. XRD analysis revealed the crystal phase of powder materials. Raman spectroscopy and XPS proved the selective separation of lithium ions. Kinetics of the process followed by pseudo-second order adsorption model with the equilibrium achieved within 12 hours. Freundlich model had the best fit with experimental isotherm data, indicating that adsorption of lithium ions on PA2200-Li<sub>2</sub>TiO<sub>3</sub> is reversible. Thermodynamic parameters

 $(\Delta G^{o}, \Delta H^{o}, \Delta S^{o})$  were calculated and indicated spontaneous endothermic adsorption process. Selectivity tests showed high selectivity of the adsorbent towards lithium ions. The composites were regenerated for three cycles and slight decrease in adsorption performance was obtained. The results of this work show that PA2200-Li<sub>2</sub>TiO<sub>3</sub> monolith composites can be successfully produced with SLS 3D-printing technology and utilized as an efficient adsorbent for lithium recovery.

## Keywords

3D-printed adsorbent lithium adsorption polyamide-Li2TiO3

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# **P.081** Formation of TiO<sub>2</sub> films with highly enhanced photoelectrochemical activity by employing spin coating, dip-coating, and high-current pulsed ion irradiation

<u>Timur Atabaev</u> Nazarbayev University, Kazakhstan

## Abstract

Photoelectrochemical (PEC) cells made from inexpensive, chemically stable, and abundant materials are critical for green hydrogen production. This study describes the successful preparation of anatase  $TiO_2$  thin films with high photoelectrochemical activity by employing a combination of spin coating, dip-coating, and high-current pulsed ion irradiation methods. We showed that spin-coated, dip-coated, and high-current pulsed ion irradiation samples yielded photocurrent densities of around 40  $\mu$ A cm<sup>-2</sup>, 180  $\mu$ A cm<sup>-2</sup>, and ~226  $\mu$ A cm<sup>-2</sup> at 1.23 V vs. RHE (reversible hydrogen electrode), respectively. A comprehensive physicochemical examination was carried out to explain a significant boost

(~5.65 times) in PEC activity. We found that high PEC activity of TiO2 films after dip-coating and high current pulsed ion irradiation processes can be attributed to a variety of factors, including decreased charge carrier recombination, improved film crystallinity, better connectivity between TiO<sub>2</sub> nanoparticles, and increased surface roughness.

## Keywords

TiO2 nanoparticles Thin films Photoelectrochemical activity green hydrogen

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# P.082 Catalyzed henry reaction by compartmentalized copper-pyrazolyl-complex modified microgels

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## Abstract

Through compartmentalization of homogeneous catalysts, the catalytic performance can be enhanced and even improve selectivity. Microgels, which are three-dimensional crosslinked polymers, serving as catalyst carriers that provide both effective compartmentalization and facilitate accessibility to the catalyst enabling the recyclability and re-usability. However, systematic study of incorporating organometallic complexes into microgels has been lacking in detailed insight in their structure and catalytic performance.

In this study, we synthesized microgels with controlled number and localization of versatile copper-pyrazolyl-complexes. [1,2] To obtain an insight into complex formation in microgels, we combined XRD and EPR studies of the copper

microgels. This comprehensive approach enabled us to identify predominant complex in the microgel and to determine complex content. Next, the catalytic activity of these microgels was evaluated in industrially relevant batch nitroaldol reactions (Henry reaction), demonstrating significantly higher yields compared to pure copper-pyrazolyl-complexes. Notably, microgels with the copper-pyrazolyl complexes localized in the core exhibited higher product yields than those with complexes in the shell. Further, the best performing microgel catalyst was used in a 200-fold continuous model process by using a tangential flow filtration (TFF) system. During this process, leaching of copper was detected, but reactivation of the microgel catalyst was achieved by copper re-loading. This resulted in significantly higher average yields over a period of 15 cycles than in the batch process.[2]

Our results demonstrate that microgel catalyst can re loaded, reactivated, and re-used in industrially relevant reactions (e.g. Henry reaction) and systems, leading to high yields.

**Acknowledgements:** The authors acknowledge funding from the German Research Foundation (DFG) through the collaborative research center SFB 985 "Functional microgels and microgel systems".

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[2] F. Grabowski et al. [manuscript submitted].

## Keywords

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F. Grabowski, V. S. Petrovskii, F. Fink, D. E. Demco, S. Herres-Pawlis, I. I. Potemkin, A. Pich, Adv. Sci. 2022, 9, 2204853.

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# P.083 Guanidine modified microgels for zinc & iron complexation as catalysts for bioplastic (De-)polymerization

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Interactive Materials, Germany, <sup>3</sup>Institute for Inorganic Chemistry, RWTH Aachen University, Germany, <sup>4</sup>Aachen

## Abstract

In recent years, microgels, a well-studied polymer system consisting of a 3D-crosslinked network, have emerged as effective catalyst carriers, enhancing activity, selectivity, and recyclability of catalytic species. These polymer networks are stimuli responsive to external stimuli depending on the monomers being utilized, wherefore they are referred to as smart carrier systems. These microgel catalysts allow compatibility within certain environments and enable reactions under reaction conditions formerly not available.

In previous studies, nanoparticles[1] and organocatalysts[2] have been incorporated into microgels and used in various catalytic reactions that open up new reaction conditions. The catalytic activity has also been retained and to a certain extent recyclability was demonstrated. Nonetheless, the incorporation of organometallic complexes into microgels lacks a systematic study, leaving gaps in understanding their structure and catalytic performance. Recently, we developed copper(II)-pyrazolyl-complex modified microgels and implemented as catalysts in a continuous Henry reaction over several cycles.[3,4]

Utilizing our gained insights from this study, we present the synthesis of guanidine-modified microgels. We then carry out complexation with zinc and iron inside the microgels to obtain the corresponding guanidine-complex modified microgels. A deliberate decision has been made to use zinc- and iron-guanidine-complexes, because of their remarkable catalytic activity in the ring-opening polymerization of lactide[5] and the depolymerization of the corresponding bioplastics[6]. Thus, the modified microgels open up new reaction conditions for polymerization and depolymerization.

**Acknowledgements:** The authors acknowledge funding from the German Research Foundation (DFG) through the collaborative research center SFB 985 "Functional microgels and microgel systems".

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## Keywords

microgels guanidine complexes catalysis (de-)polymerization

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## Full title of article

Anisotropic Microgels by Supramolecular Assembly and Precipitation Polymerization of Pyrazole-Modified Monomers

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# P.084 Predicting surfactant pKa shifts due to aggregation and ionic strength using classical simulation

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## Abstract

Modelling of surfactants is a well-established use of molecular dynamics simulations, but such simulations often neglect the dynamic nature of acid groups present in the head group of the surfactant, if the protonation state is at all considered [1]. This is of concern as it has been shown the pKa of the monomer can be significantly different from that of the pKa at the surface of a self-assembled structure, which then in turn affects the surface charge of the micelle as well as the morphology of said micelle [2]. As such we present simulations of oleic acid demonstrating a possible way of capturing this shift using recent advancements in constant pH simulations in proteins and extending them to surfactant aggregate systems, as well as those with non-zero ionic strength [3]. [1] J. J. Janke, W. F. D. Bennett and D. P. Tieleman, Langmuir, 2014, 30, 10661–10667. [2] D. P. Cistola, J. A. Hamilton, D. Jackson and D. M. Small, Biochemistry, 1988, 27, 1881–1888. [3] N. Aho, P. Buslaev, A. Jansen, P. Bauer, G. Groenhof and B. Hess, Journal of Chemical Theory and Computation, 2022, 18, 6148–6160.

## Keywords

Micelles Ionic strength Acidity

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# P.085 Investigating emulsifier effects on natural oil-based cream formulations: A study on phase behavior and stability

<u>Tania Merhi</u>, Andrea Lassenberger, Pierre Panine Xenocs, France

## Abstract

The rising consumer preference for eco-cosmetics featuring simple and natural ingredients, free from mineral oils and chemical additives, underscores a significant demand trend for natural creams. In this context, the formulation of stable emulsions is a key challenge.

This study explores the influence of emulsifiers on the formulation of creams derived from all natural ingredients and simple formulations. Through systematic variations in emulsifier content and composition, we rigorously assess their impact on phase behavior and stability. Simultaneous small-angle X-ray scattering (SAXS) and wide-angle X-ray scattering (WAXS) techniques are employed to elucidate the structural phases within the emulsions. Additionally, we investigate the kinetics of phase separation in relation to emulsifier concentrations and composition, shedding light on the temporal evolution of cream microstructures Additionally, we explore the thermal stability of these emulsions, investigating their response to temperature fluctuations and evaluating reversibility upon heating.

By providing comprehensive insights into the emulsification processes of natural oil-based creams, this study contributes to the understanding of stable natural cosmetic formulations, thereby addressing crucial needs in the eco-cosmetic industry.

## Keywords

cosmetics emulsions simultaneous SAXS-WAXS phase behavior

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Assessing suspension and infectivity times of virus-loaded aerosols involved in airborne transmission

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## All authors

Tania Merhia, Omer Atasia, Cl'emence Coetsiera , Benjamin Lalannea , and Kevin Rogera

## DOI

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# P.086 A versatile platform based on lipid vesicles to inhibit the entry of viruses into target cells

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<sup>1</sup>Department of Cytobiochemistry, Faculty of Biotechnology, University of Wrocław, Poland. <sup>2</sup>Silesian Park of Medical Technology Kardio-Med Silesia, Poland. <sup>3</sup>Acellmed Sp. z o.o., Poland

## Abstract

Humanity is confronted with a number of new, potentially deadly viruses originating from different reservoirs. Despite the greatest progress in the history of drug development, particularly in terms of the time required for the discovery and development of vaccines and other antiviral drugs and for clinical trials, there is still a great need to develop a drug platform that prevents the progression of viremia and disease, that is relatively easy to adapt to specific needs, and that can exhibit resistance to mutational variation. Our goal was to develop effective therapeutics against coronavirus and influenza infections. Using liposomes as a drug delivery platform, we focused on fine-tuning the lipid composition and size calibration procedure to achieve high homogeneity and excellent long-term stability. We were able to show that the stability of lipid vesicles depends not only on their composition, but more importantly on the size calibration technique used in their preparation. The approach based on the widely used extrusion through polycarbonate membranes makes it possible to achieve long-term stability. However, a stable and highly homogeneous formulation could also be produced by a highthroughput microfluidic homogenization technique. Liposomes bearing polyethylene glycol (PEG) derivatives were used to attach synthetic peptides to their surface to create nanostructures that recognize and deactivate viral particles. In a first step, we demonstrated the robustness and specificity of the interaction of the prepared nanostructures by measuring the kinetics of biomolecular interactions using microscale thermophoresis. The inhibitory effect of the obtained preparations against the infection of susceptible cells by pseudoviruses (lentiviruses bearing genes encoding luciferase-conjugated SARS-Cov-2 proteins) was also demonstrated. In addition, our nanoformulations showed no toxicity in vitro or in vivo. Thus, our nanoformulation can serve as a platform for virus-inactivating molecules, and versatility can be ensured by replacing individual components of the nanoformulation, such as surface-recognizing particles.

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## Keywords

liposomes molecular interactions microfluidics antiviral peptides

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Investigation of nano- and microdomains formed by ceramide 1 phosphate in lipid bilayers

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Drabik D, Drab M, Penič S, Iglič A, Czogalla A.

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# **P.087** Multifunctional lacquer coatings enriched with 2D MXene and MBene phases with antibacterial and photocatalytic characteristics

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# Abstract

Global concerns over infectious diseases transmission *via* contaminated surfaces emphasize the need for urgent solutions, especially in high-risk environments like intensive care units. Antimicrobial coatings, utilizing lacquer dispersions with synthetic resins and enhanced with engineered nanomaterials, show promise in inhibiting bacterial colonization. Despite their flexibility and convenience, coatings reported so far have limited efficacy and vulnerability to invasive bacteria. Exploring more robust alternatives is crucial to address escalating health risks associated with surface contamination.

To address this challenge, researchers propose nanomaterials like MXenes and MBenes, 2D phases composed of various transition metal carbides, nitrides, carbonitrides, and borides. Derived from parent MAX and MAB phases, synthesized multilayer structures exhibit an accordion-like morphology and can be separated into individual nanoflakes. Employed as a colloidal solution, MXenes and MBenes display unique optical and photocatalytic properties, prompting exploration for biocidal coatings. Integrated into lacquer, they release active ionic species or generate reactive oxygen species through photocatalysis when exposed to light, presenting a promising biocidal mechanism for enhanced applications.

Our study involved incorporating  $Ti_3C_2T_x$  MXene, obtained via HF/TMAOH, into lacquer formulations. We optimized MXene content to maintain the stability of colloidal lacquer dispersions, preventing nanoflakes agglomeration in coatings on opaque plastic sheets. Comprehensive investigations into morphology, MXene distribution, and optical properties unveiled a favorable band gap shift and efficient light absorption directly correlated with MXene content. These features facilitated a self-cleaning mechanism, allowing for the removal of adsorbed methylene blue coloring contaminant upon light exposure. Assessing biocidal action, the coatings displayed biostatic properties against *Escherichia coli* and *Staphylococcus aureus* in the dark environment. Further exposure to simulated daylight demonstrated nearly 100% effectiveness against both bacterial strains, showcasing remarkable self-sterilizing capabilities. Additionally, we proposed a direction for further research utilizing MBenes, developed with an HCl/H<sub>2</sub>O<sub>2</sub> approach, presenting our findings from optical properties studies of coatings. In essence, our lacquers, enriched with 2D nanomaterials, demonstrated multitasking abilities, marking a significant advancement in functional coatings for diverse applications.

## Keywords

2D Ti3C2Tx MXene Lacquer coatings Photocatalytic properties Biocidal activity

## Last published paper details

Microbiologically contaminated surfaces pose a severe threat to human health. Antibacterial coatings that effectively destroy pathogens in-situ under ambient conditions are candidates to overcome this issue. In this work, we report self-sterilizing lacquer coatings enabled by the addition of novel 2D Ti3C2Tx MXene, showing excellent photocatalytic and antimicrobial properties. The prepared facile MXene-enriched formulations based on air-drying and UV-curable lacquer dispersions were used to coat the opaque plastic sheets. The Ti3C2Tx MXene content was optimized to ensure a minimal agglomeration of flakes in a lacquer coating, as validated by stability, morphology, and structure analyses. We confirmed the uniform distribution of 2D Ti3C2Tx MXene in the coatings with energy dispersive spectroscopy (EDS) mapping. Superior optical properties of the protective lacquer coatings, added with efficient light absorption, enabled their self-cleaning from the adsorbed methylene blue coloring contaminant. This photocatalytic activity was further utilized for antimicrobial action. Under dark conditions, the protective lacquer coatings showed biostatic properties while in simulated daylight conditions, they were self-sterilizing against potentially pathogenic model bacteria such as Escherichia coli and Staphylococcus aureus. Altogether, our findings gave promise for using MXenes in daily life applications.

## Full title of article

The 2D Ti3C2Tx MXene-enabled self-cleaning and self-sterilizing lacquer coatings for offset printing

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# P.088 Maximizing photocatalytic efficiency: MBene and MXene for model and commercial dye decomposition

<u>Dominika Bury</u><sup>1,2</sup>, Michał Jakubczak<sup>1,2</sup>, Muhammad Abiyyu Kenichi Purbayanto<sup>1,2</sup>, Dorota Moszczyńska<sup>1</sup>, Agnieszka Jastrzebska<sup>2</sup>

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## Abstract

Two-dimensional (2D) nanomaterials are widely used in various applications, particularly in photocatalysis for decomposing organic compounds, owing to their unique optical properties. Among the 2D nanomaterials, transition metal borides (MBenes) and transition metal carbides or nitrides (MXenes) are outstanding photocatalysts. MBenes could be obtained from their parental ternary transition metal borides (MAB phases). In these atomically laminated bulk phases of

Colloidal form of 2D nanomaterials exhibit superior photocatalytic activity due to their high-throughput electron transfer and charge carrier mobility, facilitating the transfer of photogenerated carriers.

To obtain individual single-to-few layered MBenes, MoAlB was treating for 48 hours with an aqueous  $HCI/H_2O_2$  solution. MXene was synthesized *via* the classical HF/tetramethylammonium hydroxide (TMAOH) approach. Next, we investigated the optical properties of colloidal MBene and MXene and achieved superior results, which were utilized in the photocatalytic decomposition of model dye methylene blue. To take a step towards commercial application, we also used a commercial blend of textile dyes under simulated daylight and UV light. We achieved almost 90% effectiveness in the decomposition of dyes and demonstrated better results for MBene compared to MXene. Additionally, we observed that irradiation with 625 nm showed the highest efficiency in the photocatalysis process during analysis at various visible light ranges. The analysis of the mechanism of decomposition of dyes showed action related to surface functional groups, dye adsorption on MBenes' surface, and the activity of reactive oxygen species. Furthermore, we demonstrated that the process did not influence the material's structure and morphology. Finally, the photocatalyst was regenerated and successfully reused.

## Keywords

two-dimensional MBene two-dimensional MXene photocatalysis optical properties

## Last published paper details

Microbiologically contaminated surfaces pose a severe threat to human health. Antibacterial coatings that effectively destroy pathogens in-situ under ambient conditions are candidates to overcome this issue. In this work, we report self-sterilizing lacquer coatings enabled by the addition of novel 2D Ti3C2Tx MXene, showing excellent photocatalytic and antimicrobial properties. The prepared facile MXene-enriched formulations based on air-drying and UV-curable lacquer dispersions were used to coat the opaque plastic sheets. The Ti3C2Tx MXene content was optimized to ensure a minimal agglomeration of flakes in a lacquer coating, as validated by stability, morphology, and structure analyses. We confirmed the uniform distribution of 2D Ti3C2Tx MXene in the coatings with energy dispersive spectroscopy (EDS) mapping. Superior optical properties of the protective lacquer coatings, added with efficient light absorption, enabled their self-cleaning from the adsorbed methylene blue coloring contaminant. This photocatalytic activity was further utilized for antimicrobial action. Under dark conditions, the protective lacquer coatings showed biostatic properties while in simulated daylight conditions, they were self-sterilizing against potentially pathogenic model bacteria such as Escherichia coli and Staphylococcus aureus. Altogether, our findings gave promise for using MXenes in daily life applications.

## Full title of article

The 2D Ti3C2T MXene-enabled self-cleaning and self-sterilizing lacquer coatings for offset printing

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# P.089 Self-assembly of small-molecule fragrances and bio-surfactants in micelles

<u>Joyce Lemmer</u><sup>1</sup>, Jyoti Gupta<sup>2</sup>, Nicholas Brownbill<sup>2</sup>, Karen Edler<sup>3</sup>, Adam Squires<sup>1</sup> <sup>1</sup>University of Bath Department of Chemistry, UK. <sup>2</sup>Unilever R&D Port Sunlight, UK. <sup>3</sup>Lund University, Sweden

## Abstract

This is a study that assesses the self-assembly behaviour of bio-surfactants in the presence of small-molecule fragrances.

Fragrances are important ingredients in a wide range of surfactant-based home and personal care products. These small molecules can alter the physical properties of surfactants, such as their phase behaviour, surface tension and viscosity, and thus the final formulations' performance and stability (Fischer et al., 2009). So far, a variety of fragrance molecules with differing degrees of solubility and hydrophobicity have been studied, focusing on their solubilisation in surfactant systems, the localisation of the fragrance molecule within the surfactant micelle, and the impact of these molecules on surfactant phase behaviour (Fan et al., 2016).

The most commonly studied surfactants are of synthetic origin. However, the growing demand for renewable, naturally sourced products has resulted in an increasing need for bio-based surfactants. Produced as secondary metabolites by microorganisms, bio-surfactants offer many advantages over their synthetic counterparts: reduced toxicity, enhanced biodegradability, and higher efficacy. Primary examples of these bio-surfactants include glycolipids, more specifically rhamnolipids and sophorolipids (Nagtode et al., 2023). The self-assembly behaviour of glycolipids is well understood, but little is known about the phase behaviour of bio-surfactants in the presence of fragrance additives.

This study focuses on the characterisation of dilute solutions of glycolipids and fragrances, utilising advanced characterisation techniques such as small angle X-ray scattering (SAXS), diffusion ordered spectroscopy (DOSY), surface tension, conductivity and rheological studies. These methods are used to develop a model to predict how bio-surfactants and fragrances assemble in solution, and to compare their fundamental properties, i.e. the variation in surfactant packing parameter, the micro and nanostructure of the formulations, and their compatibility with other formulation ingredients to ultimately understand and thus evaluate their properties for use in future cleaning products.

## Keywords

Biosurfactants Fragrances SAXS DOSY
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# P.090 Tuning suspension rheology using capillary forces in water continuous systems

<u>Leonardo Ruiz Martínez</u><sup>1</sup>, F.A.M. Leermakers<sup>1</sup>, Simeon Stoyanov<sup>2,1</sup>, Jasper van der Gucht<sup>1</sup> <sup>1</sup>Wageningen University & Research, The Netherlands. <sup>2</sup>Singapore Institute of Technology, Singapore

## Abstract

An interesting phenomenon in suspensions is the tunability of its rheology by the action of capillary forces created upon small additions of a second immiscible fluid. When the capillary-driven interactions between particles form a sample-spanning network, so-called capillary suspensions are obtained. Although these systems have been studied for about a decade, they have been typically exploited using water and oil as the liquid components. Here, we demonstrate that oil-free capillary suspensions can form in aqueous two-phase systems (ATPS), that is, in water continuous systems in which segregative phase transition is induced between two hydrophilic polymers (here dextran and polyethylene glycol, PEG) (Figure 1).

Remarkably, despite the ultra-low interfacial tension characterizing ATPSs, our research shows a significant increase in storage modulus by several orders of magnitude. Validation through confocal microscopy provides clear evidence for the formation of aqueous capillary bridges and the network formation within these oil-free capillary suspensions. This study further establishes the effect of the overall polymer concentration and the quantity of the secondary phase as facile yet potent control parameters, enabling the precise modulation of the rheological response in ATPS capillary suspensions.

Beyond theoretical significance, this work shows significant potential for practical applications. The absence of an oil phase, coupled with the utilization of hydrophilic and biocompatible polymers, positions this type of capillary suspension as an optimal choice for stabilizing and structuring oil-free suspensions in pharmaceutical and food formulations.



Figure 1. (Left) Transition from liquid to gel-like behavior of aqueous suspensions upon introduction of a secondary aqueous phase formed via ATPS. (Right) Schematic picture of capillary bridges at microscopic level.

## Keywords

suspensions capillary bridges Aqueous phase separation

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# P.091 Microgel-engineered responsive microcapsules at the liquid-liquid interface for biomimetic applications

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# Abstract

Living cells consists of compartmentalized, self-assembled structures that house an array of functional moieties, allowing spatial and temporal control over the cellular activities. Sacrificial solid, gel particles and emulsion droplets (oil-in-water, water-in-oil, and water-inwater) are often employed as templates to assemble membrane-bound hollow spheres to construct artificial cell-like compartments. While the use of solid templates requires harsh methods, which restricts its use to encapsulate sensitive biomolecules, colloidal particles like rigid particles, lipids, and amphiphilic polymers are often templated onto emulsion droplets, for the formation of vesicular structures. The membrane permeability, vesicle stability, and encapsulant loading are still key barriers that need to be addressed. Herein, we focus on the engineering of uniformly distributed micro-capsules prepared by the spontaneous assembly of microgels onto emulsion droplets. Microgels are a unique class of stimuli-responsive, soft materials that share the typical properties of rigid colloids, surfactants, and macromolecules. Microgels show remarkable interfacial properties without necessarily being amphiphilic and spontaneously assemble at liquid-liquid interfaces. The study revealed that careful manipulation of the interfaces, shear force, microgel softness and surface charge resulted in soft, deformable, and robust microcapsules termed 'microgelsomes'. The microgelsomes could be dispersed in oil or water, thermally cycled to 90 °C, partially dried and rehydrated, while maintaining their structural integrity. The microgelsomes were engineered to mimic cellular functions like encapsulation, tunable membrane permeability, and programmable, membrane-gated internalized enzyme catalysis.We envision that engineering of microgelsomes with diverse functions can foster connections between non-living and living materials in novel ways.



## Keywords

Microgels protocells interfacial assembly biocatalysis

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## Full title of article

Biocatalytic self-assembled synthetic vesicles and coacervates: From single compartment to artificial cells

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Biocatalytic self-assembled synthetic vesicles and coacervates: From single compartment to artificial cells. Divya Gaur, Nidhi C. Dubey, Bijay P. Tripathi, Department of Materials Science & Engineering, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, Indi, Department of Molecular Medicine, Jamia Hamdard, New Delhi, India. 25 November 2021.

## All authors

Divya Gaur, Nidhi C. Dubey, and Bijay P. Tripathi

## DOI

# P.092 Development of peroxidase mimic nano biochar based biosensor for the colorimetric detection of hydrogen peroxide

<u>Ashmita Das</u><sup>1</sup>, Sudip Mitra<sup>1,2</sup>, Ramagopal V S Uppaluri<sup>3</sup>

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## Abstract

Colorimetric biosensors using enzyme like nanomaterial have gained enormous attention by the research community due to the ease of visual detection. In the current study, a biochar nanozyme from spent mushroom substrate has been developed for the colorimetric detection of hydrogen peroxide ( $H_2O_2$ ), which is a potent oxidizing agent or reactive oxygen species (ROS) linked to the oxidative stress in biological system. Biochar nanozyme is synthesized by a combination of slow pyrolysis-chemical oxidation-acetone extraction process. The biochar nanozyme is further characterized by XRD, FETEM, FTIR and TGA. The XRD pattern of the biochar nanozyme describes its amorphous nature. The EDS study confirms the presence of various elements especially silicon, potassium, sulphur in trace amount along with carbon and oxygen. The FETEM study discloses the morphology of the nano biochar. The nano biochar based colorimetric biosensor platform demonstrates exceptional sensitivity and specificity towards the application in visual detection of  $H_2O_2$ . The limit

of detection (LOD) of the nano biochar based platform is observed as 73 µM. Furthermore, the nano biochar based colorimetric platform is utilized for the real time detection in tap water and milk samples to ensure its practical applicability of the proposed biosensing system for point-of-care detection.

## Keywords

Nano biochar Carbon nanozyme Nanomaterial Reactive Oxygen species

## Last published paper details

1

## Full title of article

Role of modeling and artificial intelligence in process parameter optimization of biochar: A review

Journal

**Bioresource Technology** 

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All authors

Debaditya Gupta, Ashmita Das, Sudip Mitra

# DOI

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# P.093 Nitriles hydrogenation catalyzed by supported rhodium and palladium catalysts on mesoporous silica

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## Abstract

Despite recent developments in the reduction of nitriles to amines, the selective synthesis of primary, secondary or tertiary amines in simple and benian conditions remains challenging. Stoichiometric amounts of reducing agents allow the formation of amines. However, safety hazards associated with these reducing agents and their toxic by-products, and the probable contamination of the products after work-up are the major problems of such processes. Furthermore, they are not environmentally friendly and are not accepted in the concept of green chemistry. Catalytic hydrogenation of nitriles catalyzed by transition metals is an important alternative to form amines with more respect for the environment. One of the most important problems of these catalytic hydrogenations is the control of the chemoselectivity. Frequently, secondary and tertiary amines as well as Schiff bases are formed, in addition to primary amines, and purification of reaction mixtures are usually difficult. Consequently, chemoselective synthesis of amines with good yields is subject of tremendous investigations. A plethora of heterogeneous hydrogenation processes have been developed for nitrile-amine transformation. However, the preparation of the catalysts, their selectivity towards primary amines, and harsh experimental conditions are among the limitations of these methods. Catalytic homogeneous hydrogenations of nitriles to primary amines are mainly based on transition metal Pincer complexes. Unfortunately, most of these homogeneous processes are performed in costly and highly toxic organic solvents including carcinogenic and mutagenic ones. Furthermore, the separation of the catalysts from the reactions products is cumbersome, while their quantitative recovery in active form have not been performed. Also, many of these homogeneous methods are used under harsh conditions of temperature and pressure. In this presentation we wish to report a selective heterogeneous process based on mesoporous catalysts prepared by sol-gel technic for the hydrogenation of nitriles to primary amines. Excellent results were obtained, and the catalysts were efficiently recycled.

## Keywords

Nitrile hydrogenation Heterogeneous catalyst Mesoporous silica Primary amine

## Last published paper details

Abstract: Different benzylic compounds were efficiently oxidized to the corresponding ketones with aqueous 70% tert-butyl hydroperoxide (TBHP) and the catalytic system composed of CuCl2.2H2O and 2,2'-biquinoline-4,4'- dicarboxylic acid dipotassium salt (BQC). The catalytic system CuCl2/BQC/TBHP allows obtaining high yields at room temperature under organic solvent-free conditions. The interest of this system lies in its cost effectiveness and its benign nature towards the environment. Benzylic tertbutylperoxy ethers and benzylic alcohols were observed and suggested as the reaction intermediates. Analysis of organic products by atomic absorption did not show any contamination with copper metal. In terms of efficiency, CuCl2/BQC system is che catalytic systems described in the literature and which are based on toxic organic solvent. The article has 53 references that can not be included in this space.

## Full title of article

Green Organic Solvent-Free Oxidation of Alkylarenes with tert-Butyl Hydroperoxide Catalyzed by Water-Soluble Copper Complex

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## 165

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Abdelaziz Nait Ajjou and Ateeq Rahman

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# P.094 Photo-induced and microbicidal properties of spherical and rod-like colloidal gold nanostructures functionalized with methylene blue

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## Abstract

Colloidal gold nanoparticles (AuNPs) have unique photophysical properties, making them promising materials for energy transformation, harvesting, and catalysis when conjugated to organic molecules. These properties come from nanostructures' surface plasmonic resonance effect (SPR). Like AuNPs, many organic molecules absorb visible light, as is the dye methylene blue (MB) case. Photochemical properties of MB are widely studied in the fields of medicine, advanced materials, bioelectronics, and energy since such properties can be modulated by dye aggregation favored by interaction with interfaces. To improve and even obtain new photochemical properties for MB by synergism with inorganic nanomaterial photophysical properties, such as surface plasmon resonance, this study focuses on the synthesis and characterization of colloidally stable gold nanoparticles with spherical and rod-shaped morphologies, both functionalized with mercaptoundecanoic acid and methylene blue. Comprehensive characterization techniques, including UV-Vis spectroscopy, fluorescence, Fourier transform infrared (FTIR), dynamic light scattering (DLS) and high resolution transmission electron microscopy (HR-TEM) were employed to elucidate the shape, size, composition and properties of the functionalized nanoparticles. The spherical and rod-shaped colloidal gold nanoparticles exhibited distinct features in terms of size, shape, hydrodynamic radius and surface charge, as revealed by the absorption spectra, HR-TEM imaging, DLS and zeta potential measurements respectively. FTIR, in addition to UV-vis and fluorescence spectra, demonstrated the successful functionalization of the nanoparticles with mercaptoundecanoic acid and methylene blue, indicated by characteristic absorption peaks. Furthermore, the potential microbicidal effect of these functionalized gold nanoparticles under light irradiation was explored. Preliminary results suggest a light-induced antimicrobial activity, highlighting the potential applications of these nanostructures in photodynamic therapy or other light-triggered therapeutic approaches. The findings contribute to the understanding of the photo-induced properties of gold nanoparticles functionalized with methylene blue and their potential application as antimicrobial agents.

## Keywords

Gold nanostructures Methylene blue Microbicidal Photoactivity

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## Full title of article

Organic matrix-entrapped methylene blue as a photochemical reactor applied in chemical synthesis and nanotechnology

## Journal

Journal of Photochemistry and Photobiology A: Chemistry

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## All authors

de Miranda, E. G.A.; Toledo V. H.; dos Santos, C. G.; Costa, F.; Diaz-Lopez, M.; de Queiroz, T.B., Nascimento, O. R.; Nantes, I. L.

## DOI

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# **P.095** FeOF nanorod doped with Ni as a cathode for enhanced sodium-ion battery performance

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## Abstract

Sodium-ion batteries (SIBs) have emerged as an alternative to lithium-ion batteries because of their abundant reserves of sodium and low cost. Recently, intercalation-type materials such as  $Na_3V_2(PO_4)_3$ ,  $Na_7V_3(P_2O_7)_4$ , and  $NaFePO_4$  have been studied as a cathode for SIBs, but the theoretical capacities of these materials are limited to less than 150 mAh g<sup>-1</sup>. In contrast, iron oxyfluoride (FeOF) has a high theoretical capacity of 885 mAh g<sup>-1</sup>, offering promise as a cost-effective cathode material for SIBs. However, FeOF suffers from poor cyclic stability and low rate performance due to low electrical conductivity and slow ion diffusion. To solve these problems, we

attempted to synthesize FeOF with Ni doping (Fe<sub>1-x</sub>Ni<sub>x</sub>OF) to improve its structural stability and electrochemical property. The Fe<sub>0.99</sub>Ni<sub>0.01</sub>OF electrode had a reversible discharge capacity of 450.4 mAh g<sup>-1</sup> at 100 mA g<sup>-1</sup> and a low fading rate of 0.21 % per cycle after 100 cycles in the voltage range of 1.2–4.0 V. In addition, Fe<sub>0.99</sub>Ni<sub>0.01</sub>OF||hard carbon in a full cell showed a high energy density of 876.8 Wh kg<sup>-1</sup><sub>cathode</sub> with a power density of 172.8 W kg<sup>-1</sup><sub>cathode</sub> and a voltage range of 1.0–4.0 V, showing the potential as a high-performance cathode material for SIBs.

## Keywords

Sodium-ion batteries cathode FeOF Ni doping

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## Full title of article

One Dimensional Pea-Shaped NiSe2 Nanoparticles Encapsulated in N-Doped Graphitic Carbon Fibers to Boost Redox Reversibility in Sodium-Ion Batteries

## Journal

Journal of Materials Science & Technology

# Year

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## All authors

Hyunjeong Gim, Achmad Yanuar Maulana, Jiwon Choi, Jungwook Song, Boram Yun, Yuri Jeong, Nahyun An, Myeongkee Park, Cybelle M. Futalan, Jongsik Kim

## P.096 Long-range electrostatic screening and specific ion effect in zwitterionic liquids

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## Abstract

According to classical electrolyte theories, the interaction energy in dilute electrolytes decreases exponentially with distance, and the thickness of the electrical double layer increases with increasing counter-ion size and decrease with bulk ion concentration. However, recent studies have shown that concentrated electrolytes exhibit a wider range of electrostatic repulsions between charged colloidal particles than the Debye length. This under-screening is inconsistent with the Poisson-Boltzmann theory and classical correlation models for Coulomb fluids. It has been observed that there is a significant expansion of the double layer when standard electrolytes are taken at high concentrations or when salts with large ionic size asymmetries are used. To investigate how the presence of size-asymmetric buffers affects the polarization of charge around particles, we performed impedance spectroscopy highly dilute colloidal suspensions containing polystyrene microspheres in a size-asymmetric zwitterionic buffer (HEPES). The experiments were repeated using conductivity-matched phosphate buffer, and similar trends were observed in both cases. It was found that beyond a critical concentration of 0.02 w/v%, the suspensions became more resistive due to the initiation of many-body interactions, which was confirmed by scanning electron microscopy (SEM) imaging.

Nonetheless, the role of zwitterions in surface charge screening remains relatively unexplored, as laboratory studies typically use standard buffer solutions containing only a few simple salts. In this study, we investigated the combined effect of ionic and zwitterionic solutes on the interaction forces between two planar charged surfaces in these electrolytes using molecular dynamic simulations. The results indicate that zwitterions play a significant role in modifying interactions compared to simple salt solutions. We confirmed the underscreening effect in zwitterionic liquids, where they don't screen the charged surface as they layer, which strengthens electrostatic repulsions by increasing the effective surface charge.

## Keywords

size-asymmetric ions
zwitterions
Electrostatic
colloids

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# **P.097** Anti-sintering agent coatings for preventing aggregate formation during powder preparation and heat treatment

# <u>Seung-Min Yang</u>, Gyeongbae Park

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## Abstract

The Chemical Vapor Synthesis (CVS) process is a widely employed technique for producing electrode powders used in electronic components such as multilayer ceramic capacitors. This method is preferred due to its advantages in terms of high purity and crystallinity. However, CVS often results in the formation of agglomerated particles, which are undesirable as they lead to issues such as low packing density and electrical shorts.

This study introduces a novel approach called in-flight coating-assisted CVS to inhibit agglomerate formation by using coating agents. Through image analysis using field-emission scanning electron microscopy, we observed a reduction in agglomeration when employing in-flight coating in the proposed method. Additionally, we conducted heat treatment experiments on the coated metal particles. The coating agent effectively prevents sintering between metal particles during heat treatment, enabling the process even at high temperatures. Consequently, our in-flight coating-assisted CVS method yields high-quality metal powder with low agglomerates and allows for high-temperature heat treatment.

## Keywords

Metal powder Chemical Vapor Synthesis Electrode Agglomerate

## Last published paper details

J, Y. S., Abdull. S., ... & Yan. H., Swain, B. S., Lee, B., Eom, H. S., ... & Yang, S. M. (2022). Sulfur-Mediated Synthesis of Spherical Nickel Nanoparticles in a Chemical Vapor Reactor. ACS omega, 7(48), 43958-43964.

## Full title of article

Sulfur-Mediated Synthesis of Spherical Nickel Nanoparticles in a Chemical Vapor Reactor

Journal

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## All authors

Jo, Y. S., Abdullaev, M., Jin, G. H., Swain, B. S., Lee, B., Eom, H. S., Min, S. H., Kim, S. K., Kim, Y. K., Yang, S. M.

# **P.098** Wettability of waterborne and solvent-based epoxy coatings on contaminated steel panels: Surface tension and surface free energy interactions

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# Abstract

**Hypotheses:** Surface tension components, such as polar, dispersive, and acid-base contributions, can be quantified for liquid coatings, and it is expected that a coating with a surface tension lower than the surface free energy of a solid will provide adequate wettability and strong adhesion. However, under certain conditions, interactions between surface tension and surface free energy components can lead to unexpected wetting mechanisms.

**Experiments:** Adhesion of liquid epoxy coatings to oil and rust contaminated steel panels was investigated using contact angle and pendant drop measurements, as well as modelbased estimations of the ideal and roughness-corrected work of adhesion. For quantification of the theoretical wettability, the Owens, Wendt, Rabel and Kaelble (OWRK) approach, coupled with the acid-base theory, was used to determine the dispersive, polar, and acid-base components of the surface tension of liquid coatings and the surface free energy of oil and flash rust contaminated substrates.

*Findings:* Surface tension measurements of six coatings showed minimal variation, with waterborne coatings having slightly higher values. Furthermore, the roughness-corrected work of adhesion, the surface tension, and the surface free energy results, pointed to the importance of compatibility between polar, dispersive, and acid-base components in understanding wettability. Due to increased polar contributions from additives in the IQ-X EKSTRA 10W/40 engine oil, such as zinc dialkyl dithiophosphate and dimethyl sulfoxide (DMSO) extracts, coatings, contrary to expectations, demonstrated better wettability on oil-contaminated substrates. In addition, the acid-base approach was particularly useful for quantifying the wettability of non-pigmented coatings. However, estimation of the wettability through the OWRK and acid-base theories faced difficulties due to the chemical heterogeneities in pigmented coatings and the rust layer, which led to the violation of some of the underlying model assumptions.

The mechanistic understanding of this work can help to enhance coating wettability, particularly for oil and rust contaminated substrates.

# Keywords

Surface tension Surface free energy Wettability Adhesion

## Last published paper details

Cracks and defects, as a result of internal stress during curing, can accelerate the degradation and failure of protective epoxy coatings for essential infrastructures. To reduce, or eliminate, this so-called premature crack formation, it is

essential to understand the underlying mechanisms. The present work investigated the simultaneous development in internal stresses, the degree of conversion of reactants (i.e., cross-linking), the volumetric shrinkage, and the elastic modulus of a solvent-based novolac epoxy cured with a cycloaliphatic amine. In addition, the crack susceptibility of the coating was quantified from a stress–strain curve (tensile mode), and the effects of film thickness, solvent content, pigment volume concentration, and flat versus 90-degree angle geometry were mapped. Finally, digital microscopy, in combination with a nondestructive scanning acoustic microscope (SAM) analysis, proved efficient for characterization of the crack morphology. Residual solvent, due to plasticization, promotes a low crack susceptibility. Later in the process, however, the solvent plasticization contributes to a high reactant conversion, and when the solvent finally evaporates, an increased internal stress is established. This, in turn, leads to an associated higher probability for crack initiation and growth. The crack susceptibility method provides insight and input to guidelines on how to modify formulations and curing conditions.

## Full title of article

Detection and Quantification of Premature Crack Formation in Curing Epoxy Coatings

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All authors

Qiong Li, Claus Erik Weinell, and Søren Kiil

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# P.099 Functional covalent organic frameworks as sulfur host in lithium-sulfur batteries

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## Abstract

Lithium-sulfur (Li-S) batteries are considered as one of the most promising rechargable batteries due to their high theoretical energy density (2600 Wh kg<sup>-1</sup>) and lower cost. However, the dissolution and "shuttle effect" of polysulfides upon cycling in Li-S batteries can lead to the depressing cycling stability and impede their development for practical applications. Covalent organic frameworks (COFs), an emerging family of crystalline porous polymer, display high specific surface area, uniform pores with tunable size, and designable skeletons at the atomic/molecular levels. Specifically, the tunable pore properties of COFs will benefit the spatial confinement of polysulfides. The diverse functonalities may provide abandunt active sites for enhancing the conversion of discharge products in Li-S batteries (Figure 1). In this study, one organosulfur moiety (tetrathiafulvalene) is applied to construct the crystalline layered COF. A high-temperature sulfurization process allows for the formation of electron-delocalized radical backbones with decreasing bandgap, and further more active sites to facilitate the polysulfides conversion. The assembled coin cells deliver a 0.02% c



apacity fading per cycle during 1500 charge-discharge cycles at 0.5C current density.

# Keywords

Covalent organic frameworks Li-S batteries Catalysis Shuttle effect

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All authors
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# P.100 Platinum atomic layer deposition on spray-dried SiO<sub>2</sub>/iron oxide supraparticles: Tuning the activity by scaffold texture and intrinsic heating properties

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## Abstract

In the development of new emerging materials, one field of interest is the forced assembly of nanoparticles through spraydrying, creating supraparticles. By adjusting the spray-drying parameters, supraparticles provide adjustable pore sizes and surface areas, along with the combination of multiple nanoparticle functionalities. These highly porous supraparticles have a large variety of applications e.g., as temperature recorders, magnetic sensors, and hydrogen indicators.<sup>[1,2]</sup> To fabricate even more advanced materials, further functionalization of supraparticles can be accomplished via the atomic layer deposition (ALD) process.<sup>[3]</sup> ALD provides monolayer-by-monolayer material deposition, with platinum being a commonly used material for ALD. However, the combination of platinum with supraparticles through ALD is yet unprecedented. The synthesis of such new materials is shown in **Figure 1**. Supraparticles are spray-dried to generate systems with different pore sizes and surface areas. They are subsequently subjected to various Pt-ALD cycles and then tested for their catalytic activity in the reduction of 4-Nitrophenol. An increase in the pore sizes of the supraparticles is highly favored even though the active surface area and the amount of platinum are drastically reduced. This shows that diffusion and mass transport are highly important for such mesoporous supraparticle systems. Iron oxide nanoparticles are subsequently introduced to the supraparticles, allowing for additional magnetic separation and inductive heating capabilities.



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**(b)**.

Oxide

support

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Oxide

support

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Figure 1: Scheme of the synthesis of supraparticles from different nanoparticle building blocks (a) and their further functionalization with platinum via atomic layer deposition (ALD) towards catalytically active supraparticles

-CO2

-CH<sub>4</sub>

Oxide

support

Oxide

support

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# Keywords

atomic layer deposition supraparticles catalysis hydrogenation

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# P.101 Metal-organic frameworks for atmospheric water harvesting

<u>Aafaq ur rehman</u>, Parsa Amin, Alharith Yousuf, Nima Rezaei LUT University, Finland

# Abstract

Metal-organic frameworks (MOFs), a class of porous materials possesses high porosity, specific surface area, and tunable pore structures, have garnered significant interest for applications in atmospheric water harvesting, indoor humidity control, and natural gas desiccation. In this study, we investigated the dynamic sorption behavior of four different types of MOFs—MIL-101 (Cr), MOF-801, MOF-303, and Co<sub>2</sub>Cl<sub>2</sub>BTDD under high (80%) and low (40%) relative humidity conditions. The experiments were conducted within a pressure range of 2 to 5 bar and a temperature range of 25 to 50°C. Characterization of the MOFs involved X-ray diffraction (XRD), scanning electron microscopy (SEM), and BET surface area analysis. Dynamic adsorption breakthrough analysis was conducted in a column containing MOF powder (mixSorb SHP, 3P Instruments) to quantify water adsorption. At 80% relative humidity, 2 bar pressure and 25 °C temperature, MIL-101 (Cr) and Co<sub>2</sub>Cl<sub>2</sub>BTDD MOFs exhibited efficient water adsorption capacities of 0.25 g/g and 0.87 g/g, respectively. At low relative humidity (40%), MOF-801 and MOF-303 demonstrated effective adsorption capacities of 0.07 g/g and 0.16 g/g, respectively. The notably higher adsorption capacity of Co<sub>2</sub>Cl<sub>2</sub>BTDD suggests its promising potential as an adsorption material for atmospheric water harvesting, addressing the challenges posed by the global water scarcity.

# Keywords

Atmospheric water harvesting MOFs porous materials adsorption capacity

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## Full title of article

Metal-organic framework (MOF) templated hierarchical Al-doped CoxP @ graphene composite: A promising solid-state asymmetric supercapacitor with PANI derived carbon nanorods

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Journal of Alloys and Compounds

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## All authors

Emad S. Goda, Sang Eun Hong ,Bidhan Pandit, Aafaq ur Rehman, Bal Sydulu Singu, M. Shaheer Akhtar, Muhammad Sohail, Salah M. El-Bahy, Heba Gamal, Kuk Ro Yoon

## DOI

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# P.102 Surface polymerization of stearic acid adsorbed on porous calcium carbonate used as inorganic drug delivery vehicle

Helena Bach-Rojecky, Marija Mirosavljevic, <u>Damir Kralj</u>, Katarina Marusic Ruder Boskovic Institute, Croatia

## Abstract

Vaterite is a biocompatible calcium carbonate polymorph with a high specific surface area and porosity, making it a promising system for various bioactive compounds in inorganic drug delivery. When a vaterite system containing a pharmaceutical in its pores is sealed by a biocompatible coating, the release of the drug can be delayed and/or controlled. Fatty acids are biocompatible molecules with various properties and functions in the body. They consist of a straight aliphatic chain and a carboxyl group at one end. The self-assembling properties of fatty acids can be used to create responsive interfaces that can be tuned by modifying the molecular structure under the influence of pH, CO<sub>2</sub> and temperature. A monolayer of fatty acids can be further stabilized by their cross-linking into thin biocompatible polymer coating that could further delay the release of absorbed drug molecules.

In this work, we used stearic acid (SA), a saturated fatty acid with an 18-carbon chain that occurs in various animal and plant fats, to self-assemble at the surfaces of vaterite particles. The vaterite particles precipitated from the  $Na_2CO_3$ -CaCl<sub>2</sub> system were subsequently loaded with the fluorescent dye that mimics the drug molecules and then exposed to an SA solution in ethanol. Once the vaterite particles were covered with self-assembled SA molecules, they were filtered, dried and exposed to  $\gamma$ -radiation at different doses to test the extent of cross-linking. The release of the dye from the vaterite suspended in simulated body fluids (Hanks' solution) was investigated by UV-VIS spectroscopy. The systems were further

characterized by determining the hydrophobicity/hydrophilicity of the system, the surface energy and the morphological and structural properties using contact angle measurements, as well as FTIR, TGA and SEM/EDX.

## Keywords

stearic acid vaterite drug delivery gamma irradiation

## Last published paper details

Yu-Qin Niu, Jia-Hui Liu, Cyril Aymonier, Simona Fermani, Damir Kralj,\* Giuseppe Falini\* and Chun-Hui Zhou\*. Calcium carbonate: controlled synthesis, surface functionalization, and nanostructured materials. Chemical Society Reviews, 2022, 51, 7883 – 7943.

## Full title of article

Calcium carbonate: controlled synthesis, surface functionalization, and nanostructured materials

## Journal

**Chemical Society Reviews** 

Year

2022

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51

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7883

## All authors

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# **P.103** Evaluation of the promotional effect of alkali on the performance of cobalt catalyst for ethanol steam reforming process

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## Abstract

The anticipated depletion of fossil fuel reserves is turning the world's attention toward alternative energy sources. Hydrogen energy sources are considered a sustainable and environmentally friendly alternative. Among others, hydrogen can be obtained by steam reforming using ethanol from biomass conversion. This process needs an active, selective, and stable catalyst. The catalysts containing noble metals (Rh, Ru, Pt, Ir) showed superior activity and stability. However, high cost limits their industrial application, and interest shifts to catalysts based on nonnoble metals such as Co, Ni, and Cu, of which cobalt-based catalysts seem to be the most promising systems.

We aimed to develop an active, selective, and stable cobalt catalyst for steam reforming of ethanol (ESR). The catalyst's design included optimizing the alkali promotion (Na, K, Rb, and Cs) of the cobalt-based alumina-supported catalyst. The catalysts have been thoroughly characterized using spectroscopic and microscopic techniques to understand the catalytic results by determining surface-structure-activity relationships.

We obtained highly competitive (100% ethanol conversion, >90% selectivity to  $H_2$ , no  $C_2H_4$  at 500°C) catalysts based on alfa alumina. The substantial difference in the performance of undoped and alkali-doped catalysts we discussed based on

strongly affects the interaction between Co $|Al_2O_3$  catalyst and acetaldehyde. Experimental data were confronted with the results of periodic DFT-GGA+U molecular modeling (performed with VASP package). The slab models were constructed, exposing the (0001)  $Al_2O_3$  surface (with  $Al_{108}O_{162}$  stoichiometry) in contact with the cobalt cluster (Co<sub>26</sub>). It has been shown that the presence of alkali atoms is responsible for electron transfer to the metal cluster, which strongly influences the course of ESR, increasing the adsorption energy of the aldehyde intermediate and facilitating the key C-C bondbreaking step.

## Keywords

hydrogen production ethanol steam reforming cobalt catalyst alkali promotion

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Adjustment of the ZSM-5 zeolite support towards the efficient hydrogen production by ethanol steam reforming on cobalt catalysts

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G.Grzybek, M. Greluk, P. Patulski, P. Stelmachowski, K. Tarach, G. Słowik, M. Rotko, S. Valencia, F. Rey, K. Góra-Marek

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# P.104 Ultra-selective and stable ethylene detection via exsolution of catalytic Ni nanoparticles in chemiresistive gas sensors

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## Abstract

Ethylene, a gaseous indicator that provides critical information about plant aging, is biologically active in plants, even at trace levels. Therefore, it must be precisely monitored and controlled at sub-ppm levels. However, the accurate detection and clear identification of ethylene has been a major challenge, owing to its low chemical reactivity and severe embedded with exsolved Ni nanocatalysts. It completely removed interferents via catalytic oxidation and exhibited remarkable gas selectivity (approximately 60 and 32 to 1 and 0.2 ppm ethylene, respectively) and an excellent stability against humidity variations. Furthermore, owing to robust metal-support interactions in the nanocatalysts, the sensor exhibited excellent thermal stability and reliable long-term sensing performance at elevated temperatures. This study provides an approach for facilitating the successful commercialization of ethylene detectors.

## Keywords

gas sensor exsolution metal oxide catalyst Last published paper details N/A Full title of article N/A Journal N/A Year

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# P.105 Emulsions used as paint binders: Physico-chemical description of an artistic practice

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# Abstract

The search for specific artistic effects pushed major painters of the 20<sup>th</sup> century such as Otto Dix and Mark Rothko to employ egg and oil emulsions as paint binders [1,2]. Understanding the physico-chemical properties of these emulsion-based paints is key to comprehend their artistic use, yet this topic only recently gained interest of the scientific community [3,4]. Mock-up paint samples were prepared to assess the impact of the type of emulsion (water-in-oil w/o or oil-in-water o/w) and

the oil treatment (raw or partially saponified with lead oxide) on their structure, flow properties and drying mechanism. Confocal microscopy demonstrated that the structure of the emulsion is kept in the final paint, and allowed direct visualization of the location of the pigment in the binder. Rheological properties are mainly ruled by the fraction of dispersed phase, providing artists with an easy tool to tune the flow behavior of their paint, allowing them to achieve various potential visual effects. Finally, combination of NMR relaxometry and FTIR spectroscopy to follow the curing process of the paint layer highlighted major differences depending on pigment-binder interactions.



Figure: confocal microscopy images of a) an oil paint b) an o/w emulsion-based paint, with silica spheres (visible in black) as a model pigment. Red: oil phase, green: aqueous phase. Scale bar: 10  $\mu$ m. c) Flow curves and pictures of such paints prepared with lead-tin yellow as a pigment. Data are fitted with the Herschel-Bulkley model.

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[2] C. Mancusi-Ungaro, Studies in Conservation 35 (1990) 134–137. https://doi.org/10.1179/sic.1990.35.s1.028.

[3] O. Ranquet et al., ACS Appl. Polym. Mater. (2023) acsapm.3c00179. https://doi.org/10.1021/acsapm.3c00179.

[4] C. Thillaye du Boullay et al., Colloids and Surfaces A: Physicochemical and Engineering Aspects 673 (2023) 131816. https://doi.org/10.1016/j.colsurfa.2023.131816.

## Keywords

Paint Emulsion Rheology Confocal microscopy

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### Full title of article

On the way to tempera grassa: Unraveling the properties of emulsion-based paint binders

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# P.106 Physicochemical, structural and functional properties of a protein-polysaccharide complex from cashew apple bagasse

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# Abstract

The cashew tree (*Anacardium occidentale* L.) is native to tropical America and is widely available in several countries in Asia, Africa, and Central America as an economically important agricultural crop. This crucial tropical tree produces a fruit with two edible parts, including the cashew nut and the cashew apple (CA). CA is a byproduct of the cashew nut processing industry. Cashew apple bagasse (CAB), an underutilized residue of this fruit after juice extraction, is rich in vitamins, polyphenols, sugars, minerals, amino acids, dietary fiber, and proteins and can be considered a functional food.

Hence, The extraction of some techno-functional constituents from CAB and the study of their properties are therefore very relevant. The focus of this work is to characterize an extract of CAB obtained through ultrasound-assisted solubilization followed by isoelectric precipitation to assess its potential suitability for future use in food applications. Analysis of CABe composition reveals that its main constituents are proteins (22.10%) and sugars (39.49%). High-performance size exclusion chromatography (HPSEC) analysis is employed to elucidate the structure of CABe, identifying the presence of a protein-polysaccharide complex within it.

Surface properties, zeta potential, and thermal behavior are studied to confirm the presence of the protein-polysaccharide complex in CABe. The results highlight similarities between CABe and arabic gum as well as cashew gum. Therefore, CABe proves to be versatile for various food applications, such as thickening, stabilization, gelling, dispersion, water retention, emulsification, and foaming. This study concludes that, in light of the evolving trends in the food industry, the by-product of CA after juice extraction exhibits favorable functional properties. Hence, CAB can be valorized as a novel source of hydrocolloid.

## Keywords

Cashew Apple Bagasse Functional property Protein polysaccharide complex Surface property

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## All authors

M. Zié; T. Alabi; G.Karamoko; C Blecker

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# P.107 Design of polysaccharide-carriers for the release of natural actives for pest-control

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# Abstract

In the last years, the choice to use non-toxic natural substances in the place of synthetic ones is an increasing trend in many different fields. In particular, new technologies for precision farming are being developed with the goals of preserving the biodiversity and respecting the environment by reducing the use of chemicals. This approach applies to both active molecules with fertilizer, stimulating and/or pesticide properties, and carriers. In this framework, this research line aims at designing an eco-sustainable and versatile platform for the delivery of different natural actives. Sodium alginate hydrogels are promising carriers because of their low toxicity, high biodegradability and biocompatibility, the low costs of raw materials, and, last but not least, the ease of preparation and scaling-up by means of eco-sustainable methods. The hydrogel properties can be tuned in terms of stiffness and dimensions, realising a variety of possible release mechanisms,

carried out by analysing the inner local organization and dynamics by means of Electron Paramagnetic Resonance (EPR) spectroscopy, as a function of both the gelation conditions and the environmental variables (temperature, pH, presence and nature of ions). These results will be related to the hydrogel capability to encapsulate and release different natural actives, evaluated by means of spectroscopic techniques, to put the basis for the use of alginate hydrogels as a versatile precision farming technology in the agrochemical industry.

## Keywords

microgel nanogel biopesticide biostimulant

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## P.108 Green solvent-based functional ingredients prepared from oil palm empty fruit bunch

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### Abstract

Oil palm empty fruit bunch (EFB) is a major by-product of palm oil production. At present the majority of oil palm EFB is incinerated, creating environmental damage and no value. EFB represents a lignocellulosic biomass mainly composed of cellulose, hemicellulose, and lignin. This project aims to develop functional formulation ingredients from EFB utilizing green solvents and processes, focusing on the lignin component. Lignin represents the most abundant natural aromatic polymer occurring on earth. In this study, five kinds of choline chloride-based deep eutectic solvent (DES) containing carboxylic acid and ethylene glycol were prepared and successfully used to

extract lignin from oil palm empty fruit bunch (EFB). Various combinations of deep eutectic solvents (DES) were examined in their influence on extract yield and composition, lignin recovery, and wetting properties. Preliminary results on particle functionality as an oil-in-water emulsifier will also be shown. Methods included FTIR for extract composition, a chemical assay for lignin content, dialysis to remove DES chemicals following particle precipitation, and freeze-drying to obtain a final powder.

## Keywords

lignin emulsion microparticle deep eutectic solvent

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# P.109 Rhamnolipids-based oil-in-water nanoemulsions as carriers of bioactive compounds and natural colourants

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<sup>1</sup>International Iberian Nanotechnology Laboratory, Portugal. <sup>2</sup>University of Minho Centre of Biological Engineering, Portugal. <sup>3</sup>University of Coimbra, CERES, Department of Chemical Engineering, Portugal

# Abstract

Biosurfactants, such as rhamnolipids, are produced by microorganisms and are suitable for use in different areas. They became popular among scientists and industries since they present interesting characteristics, allowing them to be used as alternative emulsifiers to synthetic surfactants.

In this work, rhamnolipids were used to produce oil-in-water nanoemulsions (NEs), nanostructured lipid carriers (NLCs) and solid lipid nanoparticles (SLNs) as carriers of bioactive compounds and natural colourants. In the lipid phase, glycerol monostearate (GM) was used as a solid lipid, and medium chain triglycerides and sunflower oil were used as the liquid lipid. During the production, high shear homogenization using Ultra-turrax and ultrasounds allowed the production of nanoemulsions with sizes ranging from 100 nm to 200 nm and low polydispersity values.

Vitamin D3 (VD3) was used as the bioactive compound model, loaded in NEs, NLCs and SLNs, and characterized in terms of droplet size, polydispersity index, zeta potential, and morphology. Also, their fate under gastrointestinal digestive conditions was evaluated. The NLCs exhibited better stability and good VD3 bioaccessibility (around 60%). Regarding the colourant stability, the influence of colourant concentration and size of the emulsions on the physical properties, colour and stability. Results showed that emulsions demonstrated higher stability against aggregation and gravitational separation and minimal colour variation for the nanoemulsions with smaller droplet sizes.

This study highlights the capacity of rhamnolipids as a promising emulsifier for creating functional, coloured and stable oilin-water nanoemulsions for different applications.

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## Keywords

biosurfactant lipid-based nanosystems encapsulation emulsification

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Rhamnolipids: A biosurfactant for the development of lipid-based nanosystems for food applications

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Azevedo, M.A., Teixeira, J.A., Pastrana, L., Cerqueira, M.A.

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# P.110 Effect of tea catechins on the emulsifying properties of potato protein fractions at different pH

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# Abstract

Plant proteins, such as potato protein, are emerging as sustainable alternatives to animalbased emulsifiers to stabilize oil-in-water (O/W) emulsions, yet they present lower emulsifying capacity. In this regard, protein-polyphenol combination can lead to changes in protein structure and consequently in its functionality. This study aimed to assess the effect of catechins on the emulsification properties of two potato protein fractions, high-( $\geq$ 35kDa) and low-(≤35 kDa) molecular-weight fractions (HMWF and LMWF, respectively), at different pH. Sunflower oil-in-water (5:95) emulsions stabilized with potato protein (1.75%) at pH 3 or 7 and without or with tea catechins (0.22%) were formed and their physicochemical properties were studied. Initially, HMWF-stabilized O/W emulsions presented average droplet sizes around 500 nm, monomodal distribution and homogeneous visual appearance, regardless of pH and catechin addition. Similarly, LMWF at pH 3, either without or with catechins, rendered visually homogeneous O/W emulsions with average droplet sizes of 425 and 416 nm, respectively, and monomodal size distribution. Nevertheless, at pH 7, the average droplet size of LMWF-stabilized O/W emulsions was 4.55 µm and phase separation occurred. Interestingly, catechins helped to reduce to 1.42 µm the average droplet size of O/W emulsions stabilized with LMWF at pH 7, resulting in higher stability, as they appeared homogeneous visually. After 3 days of storage, all O/W emulsions do not present significant changes in their physicochemical properties. These findings provide novel insights into using potato protein in combination with catechins to stabilize O/W emulsions.

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# Keywords

Plant protein Polyphenol Protein-polyphenol combination Emulsification

## Last published paper details

Rhamnolipids: A biosurfactant for the development of lipid-based nanosystems for food applications

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Rhamnolipids: A biosurfactant for the development of lipid-based nanosystems for food applications

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# P.111 Advanced nanomaterials based on naphthalenediimides with applications for the energy sector

<u>Sergio Brochsztain</u>, Gabriela Oliveira, Geomar Feitosa, Tatyara Silva, Natalilian Souza Federal University of the ABC, Brazil

# Abstract

The goal of this work is to synthesize novel hybrid organic-inorganic materials based on naphthalenediimides (NDIs), with applications for the energy sector. Two new NDI derivatives were synthesized, namely, N,N'-bis(4-carboxyphenyl)-1,4,5,8- naphthalenediimide (CNDI), with carboxylate ligands, and N,N'-bis(3-triethoxysilylpropyl)-1,4,5,8-naphthalenediimide (SNDI), with condensable silane groups. CNDI was reacted with metal cations (Zn and Zr) to give metal organic frameworks (MOFs), which were incorporated in mixed matrix membranes (MMMs) for  $CO_2/CH_4$  separation. For this purpose, the NDI-based MOFs were embedded into polymer matrixes (polyetherimide / polysulfone). The permeability and selectivity of the MMMs towards different gases involved in  $CO_2$  capture were evaluated. In the case of SNDI, the potential as electron transport layer (ETL) in solar cells was evaluated. Photoinduced electron transfer from CsPbBr<sub>3</sub> perovskite nanocrystals to SNDI was observed upon irradiation, both in colloidal solutions and in thin films, indicating a great potential of the system for solar cells and photocatalysis.

# Keywords

Capture of CO2 Naphthalenediimides Metal Organic Frameworks Mixed Matrix Membranes

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Synthesis and Characterization of Two Novel Naphthalenediimide/ Zinc Phosphonate Crystalline Materials Precipitated from Different Solvents

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## All authors

Barbra Poly-Anna Vera Melo, Denis Fernando Gregório Junior, Matheus Troilo de Oliveira, Fabiane de Jesus Trindade, Jacco van de Streek, Fabio Furlan Ferreira,\* and Sergio Brochsztain

# P.112 Mechano-induced release of biomolecules from supramolecular cross-linked hydrogels for on-demand cell-activation

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## Abstract

Supramolecular interactions refer to a class of weak, non-covalent interactions, including hydrogen bonds,  $\pi$ - $\pi$  bonding or host-quest interactions. Similar to covalent bonds, they can be utilized to cross-link hydrophilic polymers chains. The resulting 3D networks are classified as hydrogels and are able to swell in a suitable solvent, typically water. Depending on the specific cross-linking strategy, the gels are responsive to certain stimuli. Thus, small variations in the environment, for instance in temperature, pH value or mechanical force are able to cause significant changes in the physiochemical properties of the gels. This responsiveness can be exploited to adjust the pore size and thus, enhance diffusion of smaller molecules within the gels, or even degrade the gels completely. Among the plethora of stimuli, mechanical stress offers immense potential in biological systems. Besides the non-invasive and non-destructive nature, it is also highly available and offers precise control over magnitude and force. The focus of this work is the development of supramolecular bulk and colloidal hydrogel systems with adjustable sizes and cross-linking densities. We investigate the loading of biomolecules (like proteins) and their mechano-triggered release kinetics in comparison to conventional covalently cross-linked hydrogels. Hereby we demonstrate that reversible host-guest complexation between β-cyclodextrin and adamantane used for dynamic cross-linking enables significantly higher control over the payload's release kinetics. Further, we utilize the biobased polysaccharide hyaluronic acid as polymer backbone. This not only ensures good biocompatibility and biodegradability, but also inherently promotes proliferation and differentiation of surrounding cells. Since there is still a lack in biocompatible carrier systems with facile control over release kinetics and low spontaneous leaching of payload, our materials offer a compelling solution to address the demand for new materials in tissue engineering and personalized medical treatment.

## Keywords

Supramolecular Chemistry Hyaluronic acid Hydrogels Mechano-responsiveness

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# P.113 Carbon quantum dot-based impedimetric sensor for cardiovascular disease monitoring

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## Abstract

Claiming 18 million lives per year, cardiovascular diseases (CVD) are the leading cause of deaths worldwide, with more than 80% of these deaths due to strokes and heart attacks. The development of CVD is mainly due to behavioral risks, including a sedentary lifestyle, tobacco smoking, and an imbalanced diet. The risk of developing CVD can be determined by monitoring a number of different biomarkers such as cardiac troponin, creatinine kinase, and d-dimer. D-dimer is a small fragment protein that is present in the blood after the degradation of fibrinogen, following a blood clot. Though d-dimer levels can be affected by a number of different factors, elevated levels are associated with higher risks of CVD.

In this study, a carbon quantum dot (CQD) based sensor was used for the detection of d-dimer. CQD is continuously gaining traction in various biomedical fields for their facile and inexpensive synthesis, excellent photoluminescence, and conductivity. The CQDs were immobilized on a screen printed electrode, resulting in a substantial increase in the conductivity of the working electrode. The CQDs were then functionalized with the d-dimer antibody. Changes in the resistance of the electrode surface resulting from the antibody-antigen interaction was measured through electrochemical impedance spectroscopy (EIS) and was well correlated with increasing d-dimer concentrations. The resulting fabricated sensor showed great sensitivity and limit of detection. The ease of its fabrication makes it an excellent candidate as a relatively inexpensive sensor for d-dimer detection.

## Keywords

carbon quantum dot antibody cardiovascular disease electrochemical impedance spectroscopy

## Last published paper details

Recent Progress in Biomedical Sensors Based on Conducting Polymer Hydrogels Jillian Gamboa, Sofia Paulo-Mirasol, Francesc Estrany, and Juan Torras ACS Applied Bio Materials 2023 6 (5), 1720-1741 DOI: 10.1021/acsabm.3c00139

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## All authors

J. Gamboa, S. Paulo-Mirasol, F. Estrany, J. Torras

## DOI

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# P.114 Nanobubble applications in medical sewage treatment for a sustainable environment

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## Abstract

Hospital wastewater poses a significant concern due to its infectious nature and the presence of diverse contaminants, including bacteria, viruses, heavy metals, disinfectants, chemicals, and drugs that pose a threat to public health. In general, wastewater encompasses the physical, chemical, and biological waste within its composition. The generation of hospital sewage is substantial, originating from various hospital units such as emergency and first aid, operating rooms, drug treatment, ICU, chemical and biological laboratories, radiology, canteen, and laundry activities. Given that hospital sewage contains potentially harmful components, its improper management poses risks to both human health and the environment by contaminating surface and groundwater. Therefore, effective treatment of hospital sewage is imperative. The primary goal of wastewater treatment plants in hospitals is to process the untreated wastewater (influent) produced by healthcare facilities before its discharge into the natural environment. The release of untreated hospital wastewater may have detrimental effects on both the environment and human health. Consequently, ensuring appropriate wastewater management within each hospital is essential. The most favorable outcomes were observed at pH 10, with degradation percentage values for COD, phenolic compounds, and total coliform reaching 91.64%, 96.15%, and 100%, respectively. Despite the superior performance at pH 10, the treatment without pH adjustment (at 7.67) still exhibited a noteworthy albeit less significant impact on degrading hospital wastewater pollutants.

## Keywords

Drug treatment Hospital sewage Microbial pathogens Hazardous waste

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Article type: Research Paper DOI: 10.30919/es8d775 Volume: 21 Article : 775 Citation: Engineered Science, 2023, 21, 775 .RIS .ENW .BIB Permissions: Copyright Number of downloads: 2668 Citation Information: 2 Description: Black cotton soil was stabilized with Polypropylene Fibers and tested for its improvement in geotechnical properties experimentally as per IS codes.

https://www.espublisher.com/journals/articledetails/775/#:~:text=The%20results%20show%20that%20polypropylene,works %20using%20this%20BC%20soil.

## Full title of article

Effect of Polypropylene Macro Fiber on Geotechnical Characteristics of Black Cotton Soil: An Experimental Investigation and Correlation Analysis

## Journal

**Engineered Science** 

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21

## First page

775

# All authors

Uday, R.A., Kiran, D., Kumar, A.G.S., Prakash, K.G., Maddodi, B.S.

# DOI

10.30919/es8d775

# P.115 Understanding the role of ionic liquid on the DNA chain morphology

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## Abstract

A new class of salts known as lonic Liquid (IL) has become an area of interest due to their unique properties such as low toxicity, high thermal and chemical stability, and high ionic conductivity. It has been found that they can be used in various applications such as DNA extraction DNA detection and can help in providing long term preservation of the DNA chains at ambient temperature. IL interacts with DNA major and minor grooves via non-electrostatic interactions, where the size of IL moieties plays an important role. Thus, it becomes important to understand the fundamental morphological change which occurs with the interaction of the DNA chains with the lonic Liquids.

In this work, DNA coated gold nanoparticle (DNA-AuNP) lattice was designed to study the effect of the IL on the DNA chain morphology. The nucleotide composite on the DNA chains were chosen to promote the formation of bcc superlattices through complimentary Watson-Crick interaction. The interparticle lattice parameters were measured at two types of lonic liquids with different carbon chain lengths. The in-situ lattice parameter estimate was obtained by using high resolution Small Angle X-ray Scattering Technique (SAXS). Further to understand the interaction mechanism of the DNA chains, the aggregation behaviour of the DNA-AuNP were studied using Tunnelling Electron Microscopy (TEM). TEM micrographs reveal the presence of clusters in DNA-functionalized gold nanoparticle (DNA-AuNP) systems. However, the configuration of these clusters is dependent upon whether the DNA is single-stranded or double-stranded. For the DNA-AuNP system consisting of a majority ssDNA, the structural transformation in DNA chain morphology is primarily dominated by electrostatic interactions. In-case of the system with a majority dsDNA, the combination of electrostatic and hydrophobic interactions controls the morphology and the extent of these forces depends upon the carbon chain of the ILs.

## Keywords

Self-assembly DNA Ionic liquid gold-nanoparticles

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Srivastava, Sunita, Anuj Chhabra, and Oleg Gang. "Effect of mono-and multi-valent ionic environments on the in-lattice nanoparticle-grafted single-stranded DNA." Soft Matter 18.3 (2022): 526-534.

## Full title of article

Effect of mono-and multi-valent ionic environments on the in-lattice nanoparticle-grafted single-stranded DNA

## Soft Matter

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- 2022

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526

# All authors

Sunita Srivastava, Anuj Chhabra, and Oleg Gang.

# P.116 Adaptive systems at air/water interface: Various approaches to stimuli-responsive Langmuir films

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# Abstract

Further development of nanotechnology requires us to move from equilibrium self-assembly to out-of-equilibrium and stimuli-responsive systems. So-called adaptive materials and systems that can adjust to external stimuli such as light, temperature, or electric field may be the next step towards advanced nanotechnology applications.

While the area of dynamic self-assembly has been developed in recent years, its application in two-dimensional systems remains unrevealed. Here, we are going to present our results on building adaptive systems at air/water interface with a Langmuir through.

Using  $Fe_xO_y@SiO_2$  nanoparticles with short N-isopropylamine oligomers grafted on their surface, we created a thermo-responsive system that is able to decrease the surface pressure with the rise of the temperature. The monolayer of the nanoparticles was able to reversibly change its morphology between disordered (at 20°C) and ordered (at 40°C) state. The introduction of the ionic force as an additional parameter allowed for further modification of the remotely controlled process of 2D aggregation.

In other studies, we show novel approaches to applying an electric field in dynamic selfassembly of molecules and nanoparticles. We propose measurement techniques that can be applied to standard Langmuir and Langmuir-Blodgett experiments that are especially useful for electric-field-driven adaptive materials. In addition, we present the formation of chains of conductive microparticles at the air/water interface in alternating electric field.

# Keywords

stimuli-responsive materials dynamic self-assembly electric field thermoresponsive systems

## Last published paper details

Zbonikowski, R.; Iwan, M.; Paczesny, J. Stimuli-Responsive Langmuir Films Composed of Nanoparticles Decorated with Poly( N -Isopropyl Acrylamide) (PNIPAM) at the Air/Water Interface. ACS Omega 2023, 8 (26), 23706–23719. https://doi.org/10.1021/acsomega.3c01862.

## Full title of article

Stimuli-Responsive Langmuir Films Composed of Nanoparticles Decorated with Poly( N -Isopropyl Acrylamide) (PNIPAM) at the Air/Water Interface

### Journal

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## All authors

R. Zbonikowski, M. Iwan, J. Paczesny

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# P.117 Induction of semi-circular stripe pattern on hydrophilic surface via gravitational pulling

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## Abstract

Solvent evaporation induced assembly of nanoscale materials is being widely explored as an alternative to other expensive techniques for manufacturing large area uniformly ordered micro and nanostructures, owing to its simple, cost-effective and widely applicable strategies. Three phase contact line (TPCL) mediated particle deposition via evaporation of colloidal droplet of gold nanorods, provides an elegant root for constructing micron and nanoscale structures with a substantial degree of tunability. This method has potential application across various fields, including biosensing, optoelectronics, printing and patterning technology. The dynamics of TPCL is pivotal in dictating the penultimate deposition pattern. Here we examined the control stripe patterns construction on hydrophilic Si substrate regulating the TPCL dynamics via gravity induced droplet shape deformation. An Asymmetrical droplet shape due to the interplay between surface tension and gravitational force leads to inhomogeneous TPCL dynamics with pinning and receding sites which assist in the fabrication of semi-circular stripe pattern. The number of stripe can be adjusted by controlling the degree of gravitational effect. The stripe formation mechanism is based on guasi-static "stick-slip" dynamics of TPCL considering the gravitational effect on the pinning-depinning behavior of the TPCL. In evaporation technique, while micron scale features mainly controlled by the fluid dynamics, the nanoscale assembly structure primarily governed by the interparticle interactions. The surface morphology of micron scale pattern and the nanoscale particles arrangement altered significantly with suspension volume which is directly related to the pinning-depinning behavior of the TPCL and interparticle interaction. Finally, the nanoscale superlattice array of plasmonic gold nanorods within the stripes were explored as molecular sensor for biomolecules such as DNA, utilizing the Raman spectroscopy technique. The ordered

assembly of gold nanorods provides a great platform for various sensing base applications in optoelectronics and nanoelectronics device fabrication.

## Keywords

Stripe pattern Stick-slip Pinning-depinning Plasmonic AuNR

## Last published paper details

Sanjoy Khawas and Sunita Srivastava. "Anisotropic nanocluster arrays to a diminished zone: different regimes of surface deposition of gold nanocolloids." Soft Matter 19.20 (2023): 3580-3589.

### Full title of article

Anisotropic nanocluster arrays to a diminished zone: different regimes of surface deposition of gold nanocolloids

### Journal

### Soft matter

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## First page

3580

## All authors

Sanjoy Khawas and Sunita Srivastava

## DOI

10.1039/D2SM01625G

# P.118 Effect of microencapsulation on the volatile composition of mustard oil

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## Abstract

Mustard oil has many phytochemicals in its composition that give it anti-inflammatory, anticarcinogenic and antioxidant properties. Furthermore, the oil has an antimicrobial function. Microencapsulation can be used to protect the active compounds of oils, in addition to ensuring a controlled release and prolonged action after application. The objective of this work was to evaluate pure mustard essential oil and mustard oil microcapsules by gas chromatography coupled to mass spectrometry (GC-MS). Mustard essential oil, donated from a company in the northwest of São Paulo, was obtained by cold pressing mustard seeds, in an extrusion press, and subsequent vacuum filtration. The microencapsulation of mustard oil was carried out by bilayer emulsification method (layer-by-layer technique), using isolated soy protein and high methoxylation pectin as encapsulants. The emulsions were prepared at pH 3.5 to guarantee electrostatic interaction between the biopolymers. The hydrodistillation technique was used to extract the mustard oil from the microcapsules and subsequent injection into the equipment, while the pure essential oil was injected directly into the equipment. Volatile compounds were evaluated by a gas chromatograph coupled to a mass spectrometer model GCMS-QP2020 (Shimadzu,

essential oil, the presence of free fatty acids and glycidyl esters predominated, while in the oil extracted from microcapsules by hydrodistillation, smaller chain free fatty acids and terpenes predominated.

## Keywords

Brassica juncea encapsulation hydrodistillation gas chromatography-mass spectrometry

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## Full title of article

Functional properties of chickpea protein-pectin interfacial complex in buriti oil emulsions and spray dried microcapsules

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Food Hydrocolloids

# All authors

Poliana Moser, Vânia Regina Nicoletti, Stephan Drusch, Monika Brückner-Gühmann

# DOI

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# P.120 Colloidally stable nano phase change slurries (NPCSs) for improved thermal energy storage fluids

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# Abstract

The production of nano phase change slurries (NPCSs) has been demonstrated that requires stable nano Phase Change Dispersions to subsequently grow a polymeric shell over such phase Change Material (PCM). That polymeric shell growth is normally carried out by colloidal chemistry routes ensuring the nanometric size of PCM capsules inside the NPCS.

We have optimized not only the sonication energy needed to produce stable NPCSs with large heat storage capacity measured by Differential Scanning Calorimetry, but also we have confirmed that a proper mixture of surfactants promotes a great colloidal stability with time and so reducing the breaking ratio. Moreover, the paraffinic material remained well

encapsulated inside a core-shell structure. With those advances the viscosity of the final nano phase change slurry (NPCS) remains low, permitting to be easily applied as heat transfer fluid in heat exchanging systems.

On the other hand, NPCSs have been implemented for the formulation of thermoregulating gypsums, being modulated the ratio of nano-encapsulated phase change material to gypsum hemihydrate ratio between 0.0-0.41. The final gypsum products showed improved thermal storage properties, lowering the thermal conductivity up to ~ 50%, and enlarging the thermal energy storage (TES) capacity in a ~ 140%, respect to the PCM-free gypsum.

In conclusion, by colloidal chemistry routes, we have demonstrated the successfully synthesis of nano phase change slurries (NPCSs) that can be implemented either in liquid state as heat transfer fluids or in a mixture to produce building materials, both pushing their base thermal properties.

## Keywords

Phase Change Material Nano Phase Change Slurries Thermal applications

## Last published paper details

Influence of the dispersion characteristics for producing thermoregulating nano phase change slurries. An environmentally friendly production of ester-biolubricant from oleic acid. Thermoregulating gypsums by using nanoencapsulated phase change material slurry. Polystyrene nanoparticles slurry as an additive for developing insulating and waterproof gypsum composites. Production of thermoregulating slurries constituted by nanocapsules from melamine-formaldehyde containing n-octadecane

## Full title of article

Influence of the dispersion characteristics for producing thermoregulating nano phase change slurries

### Journal

**Chemical Engineering Journal** 

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2022

### Volume

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139034

### All authors

D. López-Pedrajas, A. M. Borreguero, F.J. Ramos, J. F. Rodríguez, M. Jiménez-Vázquez, M. Carmona

# P.121 Influence of the acid-base properties of cobalt-based catalysts in the hydrogen production from the ethanol steam reforming

<u>Magdalena Greluk</u><sup>1</sup>, Marek Rotko<sup>1</sup>, Grzegorz Słowik<sup>1</sup>, Gabriela Grzybek<sup>2</sup> <sup>1</sup>Maria Curie-Sklodowska University, Poland. <sup>2</sup>Jagiellonian University in Kraków, Poland

## Abstract

The development and application of clean fuels such as hydrogen are the urgent task to reduce the reliance on fossil fuels. Reforming for producing  $H_2$  using small organic

economical and efficient than photocatalysis and electrocatalysis. Among different organic molecules, ethanol has generated a growing interest in recent years due to its high hydrogen content, wide availability, low cost, non-toxicity, and easy handling and storage. Moreover, ethanol has been considered a promising candidate for H<sub>2</sub> production because it can be steadily obtained from biomass through fermentation, which is environment-friendly technology. Ethanol steam reforming (SRE) has a high potential to produce H<sub>2</sub> although this process is a rather complicated one involving a wide variety of reactions, which lead to undesired by-products. Since the reaction pathway is very complex. H<sub>2</sub> vield is strongly influenced by reaction conditions and catalyst formulation. Although noble metal-based catalysts show high activity and stability in the SRE process, they are so expensive that are industrially unviable. Among transition metals, cobalt is considered to be promising for the SRE due to its ability to break the C-C bond. Co/Al<sub>2</sub>O<sub>3</sub> catalyst is a potential candidate for the SRE because of the relatively strong metal-support interaction. However, due to the support acidity, the carbon deposits derived from ethanol dehydration are formed. Also, Co/MnO<sub>x</sub> catalyst with a support which provides a spillover of oxygen species to the cobalt particles dispersed on its surface can be used in the SRE process. However, due to its basicity, MnO<sub>x</sub> favours ethanol dehydrogenation to acetaldehyde, which can also lead to carbon formation. Because the combination of MnO<sub>x</sub> and  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> could lead to the development of support materials that possess interesting mixtures of the properties of these two supports, the activity of the Co/MnO<sub>x</sub>, Co/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and Co/MnO<sub>x</sub>- $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalysts in the SRE was studied.

## Keywords

Hydrogen production Steam reforming of Ethanol Cobalt-based catalysts Catalyst deactivation

## Last published paper details

G. Grzybek, M. Greluk, P. Patulski, P. Stelmachowski, K. Tarach, G. Słowik, M. Rotko, S. Valencia, F. Rey, K. Góra-Marek, Adjustment of the ZSM-5 zeolite support towards the efficient hydrogen production by ethanol steam reforming on cobalt catalysts, Chemical Engineering Journal 467 (2023) 143239

### Full title of article

Adjustment of the ZSM-5 zeolite support towards the efficient hydrogen production by ethanol steam reforming on cobalt catalysts

### Journal

**Chemical Engineering Journal** 

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2023

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G. Grzybek, M. Greluk, P. Patulski, P. Stelmachowski, K. Tarach, G. Słowik, M. Rotko, S. Valencia, F. Rey, K. Góra-Marek

## DOI

https://doi.org/10.1016/j.cej.2023.143239

# P.122 Porous nanorods incorporated gelatin composite thermoresponsive hydrogel for NIR active drug delivery application

Snigdharani Panda<sup>1</sup>, <u>Irfan Khan</u><sup>1</sup>, Suditi Neekhra<sup>1</sup>, Sugam Kumar<sup>2</sup>, Rohit Srivastava<sup>1</sup>, Sunita Srivastava<sup>1</sup> <sup>1</sup>Indian Institute of Technology Bombay, India. <sup>2</sup>Bhabha Atomic Research Centre, India

## Abstract

Biodegradable porous nanomaterials have emerged as a promising approach for drug delivery due to their ability to encapsulate drugs, biocompatibility and their stimuli responsive properties. Gold nanorods have gained widespread recognition for their therapeutic potential, primarily owing to their chemical inertness, and tunable surface plasmon resonance. In this work, we focus on composites of thermoresponsive gelatin hydrogel and porous gold nanorods with application in drug delivery. The porous gold nanorods, (PAuNRs), synthesized in our laboratory, exhibits a strong absorbance at 750 nm and excellent photothermal efficiency of 79% on exposure with NIR laser. The encapsulation of drug loaded PAuNR in the thermoresponsive gel prevent premature drug release, enhances the therapeutic potential and ensures controlled drug release through external temperature stimuli. We find that the temperature dependent frequency sweep measurement, reveals a critical gel to sol transition of the composite gel at temperature ~ 42 °C, an important feature for drug delivery applications. The structural analysis using small angle neutron scattering (SANS), reveals the formation of a fractal like structure whose fractal dimension decreases with increase in nanorod composition. Thus, the structural studies support the observation of gel to sol transition in rheological measurements. The biocompatibility test of the new hydrogel composite is performed invitro on L929 cell and HeLa cell lines. Our results suggest that combinatorial photo and chemotherapy can efficiently kill up to 75% of cancer cell line within 24hrs. Further, we will discuss the role of bulk properties of the hydrogel composites, for application in photothermal therapy and stimuli responsive drug delivery processes.

## Keywords

Thermo responsive hydrogel Porous gold nanorod NIR-active Fractal dimension

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# P.123 Exploring efficiency and regeneration of magnetic zeolite synthesized from coal fly ash for water treatment applications

Sofi Buzukashvili<sup>1</sup>, Weiqing Hu<sup>1</sup>, Roberto Sommerville<sup>2</sup>, Ozan Kökkiliç<sup>1</sup>, Neil A. Rawson<sup>2</sup>, Philippe Ouzilleau<sup>1</sup>, Kristian E. Waters<sup>1</sup>

<sup>1</sup>McGill University, Canada. <sup>2</sup>University of Birmingham, UK

# Abstract

Industrial wastewater often contains high concentrations of heavy metals, which are known to be among the most dangerous environmental contaminants due to their toxicity and carcinogenicity.

There are various methods available to reduce heavy metal concentrations in wastewater, among which adsorption is often considered one of the most effective methods. Zeolites are known as a low-cost adsorbent for heavy metal remediation. Their unique properties, such as high porosity and surface area, ion exchange capacity, make zeolites highly suitable for water treatment.

This work explores synthesis of zeolite from coal fly ash (CFA), and investigates its effectiveness in recovering  $Cu^{2+}$ ,  $Zn^{2+}$ ,  $Ni^{2+}$ , and  $Pb^{2+}$  from an aqueous solution and the possibility for its regeneration and reuse. Moreover, to overcome the challenge of extracting fine zeolite particles from treated water, a novel method using colloidal PVA solutions to bind magnetite nanoparticles to zeolite was developed.

The results obtained in this study show that zeolite synthesized from CFA has excellent adsorption properties for the investigated metal ions in both batch and continuous flow systems. Furthermore, the results suggest that the magnetic zeolite composite can be easily separated from water using high high-intensity magnetic separator and further regenerated.

Overall, this study highlights the potential of CFA-synthesized zeolites for the removal of heavy metal pollutants from wastewater and provides insights into the mechanisms underlying their adsorption behaviour. Furthermore, it was demonstrated that the synthesized magnetic CFA zeolite has the potential for industrially relevant water treatment applications as an effective and sustainable material for the removal of heavy metal pollutants from wastewater.

## Keywords

water treatment zeolite coal fly ash magnetic zeolites

## Last published paper details

Buzukashvili, S.; Hu, W.; Sommerville, R.; Brooks, O.; Kökkılıç, O.; Rowson, N.A.; Ouzilleau, P.; Waters, K.E. Magnetic Zeolite: Synthesis and Copper Adsorption Followed by Magnetic Separation from Treated Water. Crystals 2023, 13, 1369. https://doi.org/10.3390/cryst13091369

## Full title of article

Magnetic Zeolite: Synthesis and Copper Adsorption Followed by Magnetic Separation from Treated Water

### Journal

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## All authors

Buzukashvili, S.; Hu, W.; Sommerville, R.; Brooks, O.; Kökkılıç, O.; Rowson, N.A.; Ouzilleau, P.; Waters, K.E.

## DOI

10.3390/cryst13091369

# P.124 Polysaccharide based nano-/micro-gels for the food supplements

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## Abstract

Polysaccharides, as major components of natural origin, have garnered extensive attention and utilization across diverse fields, including the nutritional manufacturing sector. Due to their advantageous properties such as safety, stability, biocompatibility, biodegradability and nontoxicity, polysaccharide-based complex systems have a significant potential in the fields of cosmetics, pharmaceutics and food engineering. Microencapsulation of active ingredients such as flavors, antioxidants, vitamins, and lipids into biopolymer nano-/micro-gels offers greater bioavailability, effectiveness, lower toxicity, and more lasting stability than conventional formulations. Therefore, understanding the physicochemical properties of these micro- and nanogels, as well as their encapsulation and release ability under various conditions, is crucial for optimizing their use in the food sector.

In this communication we present k-carrageenan and  $\lambda$ -carrageenan-based nanogels obtained as a result of electrostatic coassembly with BSA protein as macro-ionic crosslinking agent. Such systems are of interest as carriers for bioactive



Figure 1. Chemical structures of the components and effect of various pH and T condition on scattering curves of VD3 loaded and unloaded BSA-CAR system.

## Keywords

polysaccharides nanogels electrostatic complexation small-angle scattering

### Last published paper details

https://pubs.rsc.org/en/content/articlelanding/2023/py/d2py01299e/unauth

## Full title of article

Dumbbell-like polyionic complexes of dendronized poly (ethylene glycol): synthesis and self-assembly studies

#### Journal

**Polymer Chemistry** 

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2023

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14(6)

## First page

708

## All authors

Khatuntsev, S., Fanova, A., Fetin, P., Kaberov, L.I., Girbasova, N., Lezov, A.A., Zorin, I. and Bilibin, A.

# P.125 Development of Pd-based nanostructures via atomic layer deposition for cogeneration hydrogen electrolyzers

Zahra Hagheh Kavousi<sup>1,2</sup>, Clémence Badie<sup>3</sup>, Lionel Santinacci<sup>3</sup>, Massomeh Ghorbanloo<sup>2</sup>, Yaovi Holade<sup>1</sup>, Mikhael Bechelany<sup>1</sup>

<sup>1</sup>Institut Européen des Membranes, France. <sup>2</sup>Department of Chemistry, Iran. <sup>3</sup>Aix Marseille Univ, France

# Abstract

Water electrolysis for hydrogen production is an alternative renewable energy source but is inefficient and expensive. A significant portion of the electricity demand in a hydrogen production electrolyzer, almost 90%, is consumed by the oxygen evolution reaction (OER) due to its slow kinetics, requiring high electrical input.<sup>1</sup> By replacing OER with the oxidation of biomass-based compounds like glycerol (GOR), the energy input of the electrolyzer can be significantly reduced by two times. However, the most crucial obstacle in producing hydrogen fuel is to design electrocatalysts that are efficient for electrolyzers. Atomic layer deposition (ALD) is a superior method for attaining precise thickness and composition control, making it a valuable technique for growing high-quality nanostructured materials that are crucial for achieving ideal electrochemical properties.<sup>2</sup>

In this work, we report the growth of Pd-Ni-based nanostructures directly on gas diffusion electrode (GDE) by ALD and highlight the advantages of Pd-Ni bimetallic nanostructure electrodes for hydrogen evolution reaction (HER) and GOR in half-cell and in a complete electrolyzer configuration. Electrochemical characterization techniques such as cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and chronoamperometry (CA) were used to measure the electrocatalytic activity (current density, charge transfer resistance, stability, etc.). The thermal treatment to convert GDE-Pd-NiO into GDE-PdNi nanoalloys led to bimetallic-based electrodes that act synergistically and exhibit superior electrocatalytic performance: high current density at low potentials (below 1 V vs RHE) for GOR and as a reduced overpotential at the metric current density of 10 mA cm<sup>-2</sup> during HER. Additionally, EIS indicated a significant decrease in charge transfer resistance. The integration of bimetallic GDE-PdNi as positive and negative electrodes in a glycerol fueled electrolyzer resulted into an efficient and dual H<sub>2</sub> (cathode) and valuable organic molecules (anode) production system with cell voltage below 1 V, which could have significant implications for sustainable energy production.

# Keywords

Atomic layer deposition Anion exchange membrane Glycerol electrooxidation

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# Full title of article

Design of three-dimensional electrocatalytic all-in-one electrodes by leveraging electrospinning and calcination approaches

## Journal

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47

# All authors

Yaovi Holade, Zahra Hagheh Kavousi, Massomeh Ghorbanloo, Nathalie Masquelez, Sophie Tingry and David Cornu

DOI

DOI: 10.1039/d2cc05873a

# P.126 Low magnetic field effects on thin-film permalloy disks: Using transported magnetic microbeads to understand disk magnetic structure

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<sup>1</sup>Rhodes College, USA. <sup>2</sup>The University of Chicago, USA. <sup>3</sup>University of Cambridge, UK

# Abstract

Permalloy (Ni<sub>0.8</sub>Fe<sub>0.2</sub>) is a soft magnetic material capable of being magnetized and re-magnetized by low (~tens of oersted) magnetic fields. Using micro-scale permalloy thin-film disks, we can transport superparamagnetic microparticles across disk arrays in a controlled manner by applying and varying these low external fields. However, necessary for accurately describing particle motion, and in particular transitions from ordered to disordered motion, is a vortex magnetization landscape for the disks yielding stray fields that are significantly smaller than would be obtained from disks which are fully or nearly fully magnetized. In conjunction with experiments, we consider simulations based on Object Oriented Micromagnetic Framework descriptions of disk magnetization, as well as iterative simulations meant to replicate microparticle motion behavior, to investigate micromagnetic properties of the permalloy disks.

# Keywords

Magnetic Microparticles Thin Film Magnetism

# Last published paper details

I'm not clear what this means - the paper can be found at: https://doi.org/10.3390/magnetochemistry7080120

# Full title of article

Short- and Long-Range Microparticle Transport on Permalloy Disk Arrays in Time-Varying Magnetic Fields

## Journal

Magnetochemistry

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2021

## Volume

7

## First page

120

## All authors

G Vieira, E Howard, D Hoang, R Simms, D Raymond, E Cullom

# P.127 Lignin nanoparticles for developing pickering emulsions

Cristiana Pereira<sup>1</sup>, Francieli Colussi<sup>1</sup>, José Teixeira<sup>1</sup>, Lorenzo Pastrana<sup>2</sup>, Miguel Cerqueira<sup>2</sup>, <u>Michele Michelin</u><sup>1</sup> <sup>1</sup>University of Minho Centre of Biological Engineering, Portugal. <sup>2</sup>International Iberian Nanotechnology Laboratory, Portugal

# Abstract

There is a growing interest in producing sustainable material from lignocellulosic biomasses, driven by escalating environmental concerns associated with non-renewable fossil resources. The use of lignin nanoparticles (LNP) has attracted attention due to their inherent properties related to their size. These nanoparticles have demonstrated versatility in applications such as drug delivery, enhancement of barriers, reinforcement in nanocomposites, and antibacterial and antioxidant agents. Additionally, they find utility in developing Pickering emulsions, in which solid particles are used to stabilize interfaces between immiscible liquids, often described as oil and water phases, preventing droplet coalescence. This study aimed to extract lignin from lignocellulosic materials using the organosoly process and the further production of LNP and chitosan-coated lignin nanoparticles (chi-LNPs) for use as stabilizers in oil-in-water Pickering emulsions. Two conditions were applied to produce LNP from corncob (CC) lignin: CC-LNPs (0.39 mg/mL lignin) and CC-LNPs (3.3 mg/mL lignin). These exhibited a round shape, narrow size distribution, and reduced polydispersity. The LNP's chemical structure remained unaffected by production methods or chitosan incorporation. The positive charge of chitosan led to higher contact angles for chi-LNP. LNP and chi-LNP were employed to develop Pickering emulsions with various O/W ratios, yielding sizes around 10-35 µm for LNP and 19-45 µm for chi-LNP. In terms of phase separation, the LNP Pickering emulsion with a 1:99 O/W ratio exhibited 0% creaming, indicating ideal stabilization. However, for other ratios and chi-LNP Pickering emulsions, the creaming index exceeded 65%, suggesting suboptimal creaming behaviour and low stability under the tested parameters. The results highlight the potential of obtaining LNP and chi-LNP capable of producing stable O/W Pickering emulsions.

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## Keywords

lignin nanoparticles Pickering emulsions chitosan

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Separation and Purification Technology 325 (2023) 124663

## Full title of article

Lignin recovery from a mixture of SIX lignocellulosic biomasses within a biorefinery scheme based on a sequential process of autohydrolysis and organosolv

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## All authors

Rita Pontes, Michele Michelin, Aloia Romaní, Alice M. Dias, Jose A. Teixeira, Joao Nunes

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# P.128 Microparticle marvel: Self-assembly of antimicrobial peptides for controlled release of resveratrol in intestinal defense - an integrated study from *in silico* to *in vivo* approaches

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## Abstract

Food safety plays a crucial role in preventing the spread of intestinal pathogens such as Salmonella sp. and E. coli, which demonstrate resilience in various environments. Despite extensive research on antimicrobial peptides (AMPs) as effective agents against these bacteria, their efficacy is compromised in hostile conditions, including acidic pH environments. This study aimed to develop an innovative self-assembled microsystem combining an AMP with resveratrol to regulate bacterial dispersion and reduce inflammation markers through resveratrol dosage. The AMP CR2109, an analog derived from an Indian frog peptide, was synthesized using solid-phase peptide synthesis. Dispersions were prepared using a blend of 1% alginate and pectin in an aqueous solution, followed by the addition of resveratrol and AMP, and homogenization. Microparticle formation was achieved through spray drying at precise velocity and temperature settings. Results revealed the formation of self-assembled nanostructures within the colloidal dispersions of alginate and pectin, reinforcing microparticle structure due to electrostatic interactions between alginate and AMP. Molecular docking studies demonstrated the potential activity of AMP against both bacteria. In vitro intestinal release investigations showed a significant correlation between peptide and microsystem, enabling prolonged and controlled release of resveratrol, alongside gradual disintegration and liberation of AMP over time. Cell studies demonstrated no cytotoxicity in the Caco-2 line and murine macrophages. In vivo studies conducted using Galleria mellonella revealed that these microsystems are non-toxic and safe for application in inflammation caused by bacteria. Furthermore, a protective effect during gastric release was observed, with significantly efficient controlled release of resveratrol compared to conventional systems, as validated by nanodrop and HPLC. Additionally, a noteworthy increase in antioxidant activity was observed without compromising antimicrobial efficacy. These findings highlight the potential of combined alginate/pectin microparticles and AMP CR2109 to facilitate controlled release within the intestinal tract, preserve AMP antimicrobial potency, and ensure effective resveratrol delivery.

## Keywords
Antimicrobial peptide Drug Delivery System Intestinal Infections Self-assembly nanosystem

## Last published paper details

Roque-Borda, C. A., Primo, L. M. D. G., Canales, C. S. C., Caruso, I. P., de Lourenço, I. O., Colturato, V. M. M., ... & Pavan, F. R. (2024). Antimicrobial peptides grafted onto the surface of N-acetylcysteine-chitosan nanoparticles can revitalize drugs against clinical isolates of Mycobacterium tuberculosis. Carbohydrate Polymers, 323, 121449.

## Full title of article

Antimicrobial peptides grafted onto the surface of N-acetylcysteine-chitosan nanoparticles can revitalize drugs against clinical isolates of Mycobacterium tuberculosis

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# All authors

Laura Maria Duran Gleriani Primo, Cesar Augusto Roque-Borda, Christian Shleider Carnero Canales, Icaro Putinhon Caruso, Isabella Ottenio de Lourenço, Vitória Maria Medalha Colturato d, Rafael Miguel Sábio, Fernando Alves de Melo, Eduardo Festozo Vicente, Marlus Chorilli, Hernane da Silva Barud, Paula Aboud Barbugli, Henrik Franzyk, Paul Robert Hansen, Fernando Rogério Pavan.

# DOI

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# P.129 Nanoparticles Cu<sub>2</sub>O and PLGA as a drug delivery system

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# Abstract

This work analyzes the superficial and textural characteristics of  $Cu_2O$  nanoparticles synthesized by sol-gel green method, and also describes its use in the formation of a nanocomposito with plga functionalized with citrus eztract of high antimicrobial activity. By x-ray diffraction crystalline presence of  $Cu_2O$  NP was determined, nitrogen fission analysis yielded adsorption isotherms and type IV desorption with hysteresis H1, associated with mesoporous materials conglomerates with narrow pore distribution, while a band gap of 2.17 eV was determined by UV-vis spectroscopy, indicating that modifications in the synthesis process do not alter the stability or crystallinity of the material. SEM micrographs showed hexagonal structures corresponding to  $Cu_2O$  NP, which are immersed in the polymer network, FTIR spectroscopy showed stretching and bending bands corresponding to bonds derived from metal bonds and terpenes, checking for the presence of nanoparticles and extract in the nanocomposite. Regarding functionalization, 84.29 % of total

encapsulation of the extract in the nanocomposito was determined. The release profiles were performed simulating physiological conditions and monitored for 24 h, obtaining a final release of 68.61 and 80.26 % for pH 7.0 and 1.5 respectively. The Korsmeye-Peppas mathematical model describes the behavior of our liberation profiles with a quasi-fickian diffusion mechanism. These results show an improvement in the encapsulant capacity compared to other authors who have used the solvent evaporation technique for functionalization, in addition to a stabilization from the 2 h of release. The characteristics described above demonstrate that our nanocomposite is a promising system for its implementation as a nanocarrier of drugs in future research.

# Keywords

Nanoparticles Copper PLGA Drug delivery systems

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PLGA-TiO2 as a Carrier System for Drug Release

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# All authors

M. I. Torres-Ramos, M. F. Martín-Marquez, María del Carmen Leal-Moya, Suresh Ghotekar, Jorge Alberto Sánchez-Burgos, and Alejandro Pérez-Larios

# DOI

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# P.130 Polystyrene liquid-core nanocapsule synthesis via flash nanoprecipitation

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# Abstract

Nanocapsules, consisting of a solid shell and a liquid core, are an interesting class of materials with numerous applications and many different methods of synthesis. One method for the synthesis of polymer nanoparticles is flash nanoprecipitation, in which a polymer solution is rapidly mixed with a miscible non-solvent, resulting in the phase separation of the solute into nanoparticles. We report the use of this method to synthesize nanocapsules consisting of a polystyrene shell and various types of liquid cores. We show that nanocapsule formation can be described using a model in which droplets form as a result of the turbulent mixing. The diffusion of the good

solvent out of the droplets and the poorly soluble components away from the droplet interface results in the formation of the nanocapsules, with the liquid solute molecules phase separating more rapidly from the non-solvent and forming the core, while the more slowly diffusing polymer develops into an encasing shell. Particle characterization using dynamic light scattering, atomic force microscopy, and scanning electron microscopy show how liquid cores of different properties can affect the morphology and encapsulation success of the resulting nanoparticles.

## Keywords

nanoparticle flash nanoprecipitation encapsulation

### Last published paper details

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## Full title of article

Charge Transport through Superexchange in Phenothiazine–7,7,8,8-Tetracyanoquinodimethane (PTZ–TCNQ) Cocrystal Microribbon FETs Grown Using Evaporative Alignment

### Journal

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# First page

Charge transfer (CT) cocrystals, molecular crystals composed of electron donating and accepting species, are being developed for applications in optoelectronics. Here we present optical and electronic characterization of the CT cocrystal phenothiazine-tetracyanoquinodimethane (PTZ-TCNQ). This material has a broad NIR absorption peak with an optical band edge less than...

### All authors

S. Melis, S. Hung, C. Bagade, Y. Chung, E. Hughes, X. Zhang, P. Barbara, P. Han, T. Li, D. McCusker, R. Hartsmith, J. Bertke, P. Dev, I. Stone, J. Joshi, P. Vora, and E. Van Keuren

# DOI

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Katrin Zöller, Dennis To, Sera Lindner, Andreas Bernkop-Schnürch University of Innsbruck, Austria

# Abstract

Lipid-based nanocarriers are able to incorporate or adsorb exogenous and endogenous substances. Hence, different kinds of lipid-based nanocarriers including nanoemulsions, solid lipid nanoparticles and nanostructured lipid carriers with either a PEGylated or zwitterionic surface and a negative or positive charge were developed. These carriers were evaluated for their potential to interact with different hydrophilic and hydrophobic model drugs, endogenous substances and preservatives regarding substance uptake into the nanocarriers. Moreover, toxicity of the nanocarriers themselves, the substances and the combination of both was investigated on Caco2 and HeLa cells. Furthermore, cellular uptake was determined utilizing the model drugs propidium iodide and coumarin 6 in combination with the nanocarriers. Hydrophobic substances were efficiently uptaken by the nanocarriers, thereby significantly enhancing cytotoxicity. This effect was less pronounced for hydrophilic substances and preservatives. Additionally, nanocarriers provided higher cellular uptake of the model drug coumarin 6. The results provide valuable insights into the interaction of lipid-formulations with exogenous and endogenous substances and their impact on cytotoxicity.

# Keywords

Lipid-based nanocarriers Nanoemulsions Solid lipid nanocarriers Nanostructured lipid carriers

## Last published paper details

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Fluorescent hydrophobic ion pairs: A powerful tool to investigate cellular uptake of hydrophobic drug complexes via lipidbased nanocarriers

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# All authors

Katrin Zöller, Anna Karlegger, Martyna Truszkowska, Daniel Stengel, Andreas Bernkop-Schnürch

# P.132 Limited cellular uptake of liposomes: Might thiolated phospholipids hold the key?

<u>Daniel Stengel</u><sup>1</sup>, Zeliha Duygu Özdal<sup>2</sup>, Martyna Truszkowska<sup>1</sup>, Ahmad Saleh<sup>1</sup>, Andreas Bernkop-Schnürch<sup>1</sup> <sup>1</sup>University of Innsbruck, Austria. <sup>2</sup>Erzincan Binali Yildirim University, Turkey

# Abstract

Aim: It was the aim of this study to evaluate the impact of surface thiolation on cellular uptake of liposomes.

of liposomes were investigated. Cellular uptake studies were performed on Caco-2, HeLa, HEK and SW620 cells, involving both quantitative analysis through flow cytometry and qualitative evaluation via confocal microscopy. Additionally, we investigated the impact of an oxidizing agent on thiol-dependent uptake

Results: Blank and thiolated liposomes exhibited a size of 149 nm to 274 nm and a PDI between 0.3 and 0.45. Liposomes were stable in simulated intestinal and gastric fluid. Hemocompatibility studies and cytocompatibility studies of liposomes showed negligible toxic effects of liposomes. Cellular uptake of thiolated liposomes was 1.8-, 5.4-, 2.1- and 1.4-fold enhanced in comparison to blank liposomes on Caco-2, HeLa, HEK and SW620 cells, respectively. The results were qualitatively verified by confocal microscopy. Thiol dependent uptake was influenced by oxidizing agents on HeLa cells.

Conclusion: Surface thiolation represents a promising approach to enhance cellular uptake of liposomes.

### Keywords

liposomes thiolated phospholipid cellular uptake confocal microscopy

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## Full title of article

The power of sulfhydryl groups: Thiolated lipid-based nanoparticles enhance cellular uptake of nucleic acids

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### All authors

Daniel Stengel, Arne M. Jörgensen, Ilaria Polidori, Paul Kapitza, Fabrizio Ricci, Andreas Bernkop-Schnürch

# DOI

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# P.133 Introduction of a phosphate-releasing surface in mixed micelles: Advanced approach for oral drug delivery

Annika Postina, Daniel Stengel, Andreas Bernkop-Schnürch University of Innsbruck, Austria

### Abstract

**Hypothesis:** Mixed micelles of phosphorylated and cationic surfactants provide synergistic effects to overcome the mucus and epithelial barrier for improved oral drug delivery.

**Experiments:** Mixed micelles were formed using the anionic and phosphate ester-containing surfactant C12-15 alcohol 3 ethoxylate phosphate ester (PME) as well as the cationic surfactant 1,2-Dioleoyloxy-3-trimethylammonium-propane chloride (DOTAP). Molar ratios of 90:10 and 80:20 (PME:DOTAP) were used along with pure PME micelles. Micelles were

porcine intestinal mucus before and after the treatment of micelles with IAP. Furthermore, cell viability and cellular uptake were investigated on Caco-2 cells.

**Findings:** The CMC for PME was determined to be 0.61 mM, while for 90:10 (PME:DOTAP) and 80:20 (PME:DOTAP) it was 0.85 mM and 0.80 mM respectively. Phosphate release increased with both isolated and cell-associated IAP in the following order: 80:20 (PME:DOTAP) < 90:10 (PME:DOTAP) < PME. Significant decrease in phosphate release was observed during micelle incubation without isolated IAP or when co-incubated with Caco-2 cells and alkaline phosphatase inhibitor cocktail II (PIC II). Regarding mucus permeability, PME micelles demonstrated the highest permeability, with 28% dye permeation after 4 hours, followed by 90:10 (PME:DOTAP) with 22% and 80:20 (PME:DOTAP) with 20%. All formulations were not toxic in concentrations below, at and above the respective CMC, as cell viability remained > 90%. The Cellular uptake of fluorescent dye was improved 10-fold by 80:20 (PME:DOTAP) and 15-fold improved by 90:10 (PME:DOTAP) compared to PME micelles.

**Conclusion:** The findings of this ongoing study provide promising evidence that mixed micelles containing phosphorylated and cationic surfactants exhibit not only enhanced mucus permeation capacity but also improved cellular uptake.

## Keywords

Micelles Oral Drug Delivery Phosphate-release Cellular uptake

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# All authors

N/A

# P.134 Spatially controlled photothermal crosslinking for the realization of a photosensitive hydrogel scaffold able to modulate the activity of a 3D neural network

<u>Andrea Andolfi</u>, Donatella Di Lisa, Alberto Lagazzo, Sergio Martinoia, Laura Pastorino University of Genoa, Italy

# Abstract

Recent years have seen a growing focus on neuromodulation as a critical element in understanding neural mechanisms and improving therapeutic strategies for neural disorders. Thermoplasmonic modulation, mainly using gold nanoparticles, stands out among various techniques due to its advantages, such as enhanced spatiotemporal resolution, minimal invasiveness, and deep tissue

Current in vitro models using thermoplasmonic neuromodulation are mostly limited to two dimensions and rely on animal cells or scaffolds that are poorly biomimetic. However, recent research has demonstrated the potential of a chitosan-based thermogel to accurately mimic brain tissue's mechanical properties, enabling the development of a three-dimensional, long-term functional neural culture. Inspired by this model, our study proposes a novel method involving spatially controlled photothermal fabrication to create a photosensitive thermogel for the activity modulation of a three-dimensional neural culture.

We obtained cortical neurons from human induced pluripotent stem cells, which we resuspended with astrocytes inside the polymeric solution. The thermosensitive polymeric solution is functionalized with gold nanorods, acquiring optical properties fundamental to control the crosslinking process. Gold nanorods facilitate precise heat release, triggering crosslinking and forming a photosensitive scaffold that accurately replicates the shape of the near-infrared laser spot used for irradiation. Thanks to its plasmonic properties, the photosensitive scaffold obtained can modulate the activity of the embedded 3D neural network.

Based on our research findings, the photosensitive ink offers a promising alternative for digital light processing, replacing conventional inks that utilize photoinitiators and UV-light, which can be harmful to cells. Additionally, the photosensitive scaffold produced has the potential to contribute significantly to the advancement of research on neural networks, ultimately facilitating a more profound comprehension of intricate brain functions and disorders.

# Keywords

Photothermal hydrogel crosslinking 3D neural culture Gold nanorods Neuromodulation

## Last published paper details

A. Andolfi, P. Arnaldi, D. Di Lisa, S. Pepe, M. Frega, A. Fassio, A. Lagazzo, S. Martinoia, L. Pastorino, A micropatterned thermoplasmonic substrate for neuromodulation of in vitro neuronal networks, Acta Biomater 158 (2023) 281–291. https://doi.org/10.1016/j.actbio.2022.12.036.

## Full title of article

A micropatterned thermoplasmonic substrate for neuromodulation of in vitro neuronal networks

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# All authors

A. Andolfi, P. Arnaldi, D. Di Lisa, S. Pepe, M. Frega, A. Fassio, A. Lagazzo, S. Martinoia, L. Pastorino

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# P.135 Green-based multitarget nanoformulations to prevent biofilm contaminations in nosocomial environments

<u>Giovanni Lo Bello</u>, Roberto Raiteri, Laura Pastorino, MariaLuisa Cristina, Orietta Monticelli, Elena Dellacasa University of Genoa, Italy

# Abstract

Nosocomial infections or healthcare-associated infections (HAIs) refer to infectious diseases acquired in a health facility. These infections are mainly due to the spread of a pathogen agent into a vulnerable host and pose an important cause of mortality, morbidity, prolonged hospitalization, and increased treatments with antimicrobial agents. Among the pathogens involved in HAIs, it has been observed that bacteria can adhere to surfaces and aggregate forming a complex structure, called biofilm, which makes them much less sensitive to external agents. Bacterial biofilms are difficult to manage because they consist of organized bacterial cells within a self-produced extracellular matrix, which secures them to surfaces, shields them from external threats, and promotes their growth and spreading to other areas. From this scenario, the urgent need to explore innovative strategies for treating biofilm infections arises.

This project aims to develop a multitarget nano-platform capable of degrading bacterial biofilm and killing dispersed cells. More in detail, an attempt was to functionalize nanoparticles, based on chemically-modified PCL, in two ways: some of them were loaded with quercetin, for antibacterial activity, and others were functionalized by using the enzyme alpha-amylase to break down the bacterial biofilm.

Subsequently, the functionalized nanoparticles were characterized through various analyses (SEM, AFM, DLS, etc). Furthermore, the effectiveness of the treatment was tested on four different strains of *Staphylococcus aureus* biofilms. The results indicate that the nanoparticles maintain a regular spherical shape over time and demonstrate a significant capacity to remove *Staphylococcus aureus* biofilms. The success of this project would pave the way for the search for new innovative strategies useful for reducing contamination and therefore nosocomial infections, making the treatment path safer and, above all, saving time, money, and forces on the part of healthcare facilities.

# Keywords

Nanoplatform Bacterial Biofilm Atomic Force Microscopy Healthcare Associated Infections

# Last published paper details

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# Full title of article

Surface Properties of a Biocompatible Thermoplastic Polyurethane and Its Anti-Adhesive Effect against E. coli and S. aureus

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Elisa Restivo, Emanuela Peluso, Nora Bloise, Giovanni Lo Bello, Giovanna Bruni, Marialaura Giannaccari, Roberto Raiteri, Lorenzo Fassina, and Livia Visai

# DOI

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# P.136 A new centrifugal setup for measuring the strength the adhesive contact of ice with solid surfaces

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## Abstract

Adhesion of ice, formed as a result of freezing of water precipitations, significantly affects the material performance in outdoor conditions and causes various complications, such as ice accretion on aircraft and helicopter structures, the increased accident rate of vehicles, human casualties during transportation by sea and river transport, failure of electric power lines etc. The adhesive strength of contact between ice and solid quantitatively characterizes the force that must be expended to separate a unit area of such contact. Knowledge of this characteristic is very important in many applications for assessing the effectiveness of measures taken to combat icing on the surfaces of aircraft, air navigation equipment, wires and structures of overhead power lines. We present a new experimental setup which provides a comprehensive tool for obtaining the statistically supported values of shear adhesion strength of ice to test surfaces in well-defined experimental conditions.

The breakthrough advantages of this setup are related to:

-stroboscopic illumination which allowed accurately measure (not calculate) the rotation speed for each ice detachment;

-the possibility to measure ice adhesion strength for 24 samples simultaneously and in identical conditions, which results in obtaining the statistically reliable value;

- performing the whole experiment from water freezing to fracture of contact between the ice and the solid inside the climatic chamber with precise temperature control, which allowed excluding from the consideration the misleading values of ice shear stress due to local temperature increase in the region of ice/substrate interface, and avoiding other possible perturbations related to transfer of iced samples from freezing device to measuring tool.

After introducing the setup, we will briefly discuss some important experimental regularities in the behaviour of ice adhesion to different solid substrates with variation in temperature, conditions of ice formation, exposure to environment and regimes of testing.

# Keywords

Ice adhesion Antiicing surfaces Measurement technique Superhydrophobicity

### Last published paper details

1. Ludmila B. Boinovich, Alexandre M. Emelyanenko, Recent progress in understanding the anti-icing behavior of materials. Advances in Colloid and Interface Science 323 (2024) 103057

Recent progress in understanding the anti-icing behavior of materials

# Journal

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# All authors

L.B. Boinovich, A.M. Emelyanenko

# DOI

10.1016/j.cis.2023.103057

# P.137 Dynamic interfacial tension measurement across various time scales using multiple methods

<u>Boxin Deng</u>, Tatiana P. Santos, Meinou Corstens, Karin Schroën Wageningen University, The Netherlands

# Abstract

Emulsions and foams are common product forms in food, pharma, and cosmetics. For these products to be stable, the interface of either droplets or bubbles needs to be stabilized through adsorption of surface-active components. The adsorption is reflected in the (dynamic and equilibrium) interfacial tension and viscoelasticity, which determine not only short-term, but also long-term stability of droplets and bubbles. Especially, during the short times needed for droplet/bubble formation, the stability of an emulsion (or foam) is determined by dynamic adsorption, which makes it crucial to understand adsorption at the typical time scale of droplet/bubble formation. The actual time scales depend greatly on the dispersion technique and conditions used. In a colloid mill, droplets are formed at time scales in the range of 0.1-1 s, while in a high-pressure homogeniser, the relevant time scales are 0.1-30 ms, which makes the measurement of dynamic interfacial tension challenging.

Monitoring dynamic adsorption at (sub)millisecond time scales is not possible with the classical droplet volume tensiometer (DVT), with which after starting the measurement, the acquisition of dynamic interfacial tension starts only when a drop/bulb with the pre-defined volume is formed at the tip of the needle, which usually takes a few seconds. For bubbles, the bubble pressure tensiometer (BPT) and microfluidic tensiometer (e.g., our EDGE tensiometer,) are able to access the dynamic interfacial tension at time scales down to 0.1 ms; for droplets, the EDGE tensiometer can access time scales down to 1 ms. In this presentation, we make a thorough comparison among these techniques, concerning the measurement principle, the properties (type and concentration) of the surface-active components, and the interface (e.g., gas/liquid and liquid/liquid). The obtained insights allow extending these techniques to cover short and long time scales.

# Keywords

microfluidics dynamic interfacial tension short time scales proteins

## Last published paper details

Deng, Boxin, Karin Schroën, and Jolet de Ruiter. "A microfluidic study of bubble formation and coalescence tuned by dynamic adsorption of SDS and proteins." Food Hydrocolloids 140 (2023): 108663.

## Full title of article

A microfluidic study of bubble formation and coalescence tuned by dynamic adsorption of SDS and proteins

## Journal

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# All authors

Boxin Deng; Karin Schroën; Jolet de Ruiter

# DOI

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# P.138 "Synergistic effect" based novel and ultrasensitive approach for the detection of serotonin using DEM-modulated bimetallic nanosheets

Deepak Dabur

National sun yat sen university, Taiwan

# Abstract

Neurotransmitters have been of immense scientific interest due to their importance as human-health biomarkers. Several reports suggest necessary improvisations in the sensing capabilities of these neurotransmitters. Herein, the authors report a novel synthesis methodology for bimetallic aluminum–tungsten (Al–W) nanosheets, with the hybrid nanostructure showing high specificity toward serotonin neurotransmitters. The inspiration to design hybrid metallic nanosheets depends on the inherited optical properties of the parent precursors. The interstate conversion (ISC) between Al–W nanosheets promoted photoluminescent behavior with serotonin. The PL study shows that serotonin drastically enhanced lem at 335 nm. The importance of emission below the visible spectrum is to modulate any possible aggregation-induced emissions, which earlier troubled analytical chemists. The understanding of the selective detection of serotonin from a group of similar neurotransmitters is discussed with nanomolar quantification. The quantified detection limit using Al–W nanosheets is 0.05 nm with high linearity (R2 = 0.9906). Furthermore, real-world quantification studies have been performed on human urine and serum samples with R2 of 0.9938 and 0.9801, respectively.

# Keywords

Bimetallic fluorescence serotonin Synergistic effect

Last published paper details

Two-dimensional ion–molecule chelation reaction (2D-IMCRs) to form a two-dimensional dual optical sensor (2D-DOS): synthesis and application of Phen-SnO 2 nanosheets for the fluorometric and colorimetric sensing of nitroaromatic explosives D Dabur, YT Chan, HF Wu - Environmental Science: Nano, 2023

# Full title of article

Two-dimensional ion–molecule chelation reaction (2D-IMCRs) to form a two-dimensional dual optical sensor (2D-DOS): synthesis and application of Phen-SnO 2 nanosheets for the fluorometric and colorimetric sensing of nitroaromatic explosives

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# All authors

Deepak Dabur, Yen-Ting Chan, Hui-Fen Wu

# DOI

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# **P.139** Physicochemical evaluation of κ-carrageenan/hydroxyapatite composites as bioinks for extrusion-based bioprinting applications

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# Abstract

Bioprinting has emerged as a revolutionary technology which involves three-dimensional printing of tissue constructs using cells. Extrusion-based bioprinting in particular represents one of the most widely used techniques due to its simplicity and diversity. It necessitates the use of inks with shear thinning properties to reduce the shear stress applied to cells as well as high viscosity to retain stability of the printed construct. For this purpose, different types of biopolymer-based hydrogels and their composites with bioceramics and bioglasses have been used as bioinks due to their shear thinning and high biocompatibility properties.

 $\kappa$ -Carrageenan ( $\kappa$ -CA), a naturally occurring polysaccharide, is well known for its similarities with glycosaminoglycans. It exhibits shear-thinning and thermo-reversible gelation behavior. To improve shape fidelity of  $\kappa$ -CA-based 3D tissue constructs, methacrylation of the  $\kappa$ -CA backbone has been a general approach to obtain a chemically crosslinked final construct. Here, composites of methacrylated  $\kappa$ -CA-MA and HAp were systematically investigated as a promising bioink for osteochondral tissue engineering applications.

For this purpose,  $\kappa$ -CA-MA with different methacrylation levels, low ( $\kappa$ -CA-L-MA), medium ( $\kappa$ -CA-M-MA), and high ( $\kappa$ -CA-H-MA) were synthesized and their methacrylation degree as well as chemical structure were evaluated by <sup>13</sup>C-NMR and FTIR analyses, respectively. The rheological properties of the prepared bioinks were evaluated as a function of methacrylation degree and HAp content by performing amplitude shear sweep tests and temperature sweep tests. Methacrylation was found to directly affect the shear thinning property and thermoresponsivity of  $\kappa$ -CA due to changes in the amount of hydrogen bonds. Additionally, ionic interfacial interactions between the  $\kappa$ -CA sulfate group and the HAp surface were found to dictate final rheological properties of the composite bioink in terms of viscosity, storage modulus, and gel point.

# Keywords

Bioprinting Composite bioink κ-Carrageenan/Hydroxyapatite Functional interfaces

## Last published paper details

Chitosan/PVA reinforced boron/strontium multi-substituted hydroxyapatite-based biocomposites: Effects of synthesis pH and coating on the physicochemical, mechanical, and in ... S Kansız, MT Vurat, M Parmaksiz, AE Elçin, YM Elçin Materials Today Chemistry 35, 101865

# Full title of article

Chitosan/PVA reinforced boron/strontium multi-substituted hydroxyapatite-based biocomposites: Effects of synthesis pH and coating on the physicochemical, mechanical, and in vitro biological properties of scaffolds

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# All authors

Seyithan Kansız, Murat Taner Vurat, Mahmut Parmaksiz, Ayşe Eser Elçin, Yaşar Murat Elçin

# DOI

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# P.140 Construction of high-density polyelectrolyte patches on the hydrogel to accelerate solar vapor generation

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# Abstract

Solar-driven water generation, which can separate the soluble or dispersed contaminants from water, is particularly desirable due to its green energy utilization for water purification. Here, we present a concept to enhance solar vapor generation by surface-modifying the hydrogel with high-density polyelectrolyte patches by electric field-driven grafting. In the first system, the micelles with hydrophobic polystyrene (PS) core and quaternized P4VP (QP4VP) polyelectrolyte shell were prepared. Under the electric field, the high-density QP4VP on the shell of the micelles were pulled towards and entangled with the hydrogel (the mesh size of hydrogel is much smaller than PS core) while strong repulsion between micelles favored their uniform distribution, in which QP4VP block chains were extensively entangled with the hydrogel with the hydrogel surface. Extensive entanglement between QP4VP on the shell-forming

hydrogel *via* osmotic pumping. Meanwhile, the methyl groups connected to the quaternized pyridine group of QP4VP weaken the hydrogen bonding between water clusters, facilitating water evaporation. As expected, high-density QP4VP micellar surface-modified hydrogels greatly accelerated solar vapor generation even without photothermal nanoparticle embedding. Furthermore, the amphiphilic Janus patches modified surface with tens of nanometers in thickness was prepared by selectively dissolving the non-entangled PS-*b*-QP4VP in the micelles. The Janus patches have PS domains on the top of dozens of QP4VP block chains, in which QP4VP was extensively entangled with hydrogel. Similarly, the Janus patches surface-modified hydrogel exhibited excellent stability and fast solar vapor generation. More importantly, the surface coverage of hydrophobic domains promoted the further reduction of salt ion rejection in the purified water.

# Keywords

High-density polyelectrolyte core-shell micelle amphiphilic Janus patch solar vapor generation

## Last published paper details

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# P.141 In-situ generation of stem cell culture-based bioactive extracellular matrix hydrogel on synthetic tissue engineering scaffolds

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# Abstract

Tissue engineering (TE) is a regenerative medicine field that aims to develop in-vitro biological equivalents of damaged or lost tissues. Its success depends on the appropriate use of tissue-specific cells, bioactive molecules and special threedimensional (3D) structures called scaffolds. Among other critical components, cells have ceased to be a limitation by the introduction of stem cells with their unique properties and source diversities. On the other hand, an optimal scaffold that can mimic structural and bioactive components in-vitro has not been developed to date. The inimitability of the complex and unique composition of the native extracellular matrix (ECM) and the inadequacy of scaffolding materials used for final products have generally fallen short of providing the complex bioactivity of native ECM, a bioscaffold that evolves at embryonic stages.

This study aims to overcome the limitations encountered in ECM-mimetic scaffold productions by developing synthetic biomaterials modified with cell culture-derived ECM. In the first stage, 3D poly(ε-caprolactone) (PCL) scaffolds with optimal pore size and interpore connections were fabricated using the salt leaching technique and extensively characterized (SEM, micro-CT, mechanical, porosity, etc.). Next, stem cell culture-based bioactive ECM hydrogel was incorporated into PCL scaffolds via decellularization. In the last stage, the ECM composition and bioactive factor contents of the biohybrid constructs were investigated. The findings revealed that biohybrid scaffolds had interconnected pores with desired size and suitable mechanical strength for subsequent in-vitro/in-vivo studies. The findings also demonstrated the successful incorporation of cell-derived ECM hydrogel into scaffolds with natural bioactive contents.

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# Keywords

ECM hydrogel Bioactive scaffold Cell culture-derived ECM Tissue engineering

## Last published paper details

Bioactive composite hydrogels as 3D mesenchymal stem cell encapsulation environment for bone tissue engineering: in vitro and in vivo studies Vurat MT, Parmaksız M, Elçin AE, Elçin YM Journal of Biomedical Materials Research Part A, 111, 261-277 (2023) DOI: 10.1002/jbm.a.37457

### Full title of article

Bioactive composite hydrogels as 3D mesenchymal stem cell encapsulation environment for bone tissue engineering: in vitro and in vivo studies

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# All authors

Vurat MT, Parmaksız M, Elçin AE, Elçin YM

# DOI

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# P.142 Decellularized ECM hydrogel and bioceramic nanoparticles-based mechanically reinforced biomaterial for tissue interface repair

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### Abstract

Biopolymers & bioceramics are widely used biomaterials in orthopedic tissue repair. Using these biomaterials, it is possible to produce homogeneous tissue scaffolds with well-known chemical & biological compositions of bone or cartilage. However, challenges arise in reconstructing heterogeneous tissues, e.g. calcified cartilage at the bone-cartilage interface or entheses at the tendon-bone interface. These interfaces have unique differences in organization, composition & mechanical properties than the individual tissue types forming them. Traditional biomaterials fall short of successfully mimicking the bioactive components of the extracellular matrix (ECM) (proteoglycans, surface proteins & growth factors). On the other hand, decellularization, has brought the opportunity to harness natural tissues as biological scaffolds. The main aim here is to provide biocompatibility while preserving the complex bioactive ECM components via decellularizing tissues/organs. It is noteworthy that studies using decellularization technology in the repair of interfaces are limited.

In this study, the aim was to develop mechanically-reinforced regenerative composite hydrogels for both enthesis and calcified cartilage tissue interfaces. In the first part of the study, tendon & cartilage tissues of bovine origin were decellularized by optimization of decellularization protocols. After determining the decellularization efficiencies of the applied processes, ECM-based biological hydrogels were produced via enzyme digestion & their characterization was carried out comprehensively. In the second step, nanohydroxyapatite was incorporated into the hydrogels to mechanically reinforce & chemically mimic the target interface tissues. The findings revealed that cellular components of native tissues could be removed while successfully preserving their natural bioactive contents, such as sulfated glycosaminoglycans, collagen etc. It was determined that the thermal stability & compressive strength of the resulting biocomposites increased significantly by incorporating bioceramic nanoparticles into hydrogels. Additionally, all produced scaffolds were found to be highly biocompatible & hemocompatible.

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### Keywords

ECM hydrogel Composite Tissue Interface Calcified cartilage

### Last published paper details

Parmaksiz, M. (2022). Decellularized tendon-based heparinized nanocomposite scaffolds for prospective regenerative applications: Chemical, physical, thermal, mechanical and in vitro biological evaluations. Journal of the Mechanical Behavior of Biomedical Materials, 134, 105387.

### Full title of article

Decellularized tendon-based heparinized nanocomposite scaffolds for prospective regenerative applications: Chemical, physical, thermal, mechanical and in vitro biological evaluations

#### Journal

Journal of the Mechanical Behavior of Biomedical Materials

#### Year

2022

#### Volume

134

### First page

105387

All authors

Mahmut Parmaksiz

# P.143 The effect of GF-20 modified-HAp on the physicochemical properties of PLA/HAp composites

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# Abstract

Poly(lactic acid) (PLA) has found extensive application in orthopedic and dental fields for hard tissue applications. Nonetheless, PLA lacks the capability to directly bond with bone, thereby restricting its potential applications. Hydroxyapatite (HAp) is the most frequently used bioceramic to improve osteoconductivity and osteoinductivity of PLA. However, PLA/HAp composites suffers from unfavoured interfacial interactions between PLA matrix and HAp surface. To minimize this incompability between PLA and HAp surface, surface modification approaches have been a promising approach. In this study, (3-triethoxysilylpropyl)succinic anhydride (GF-20)-modified HAp particles (F-HAp) were synthesized and then incorporated into the PLA matrix to prepare PLA/F-HAp composites. The interface interactions of the obtained composites were elucidated by FTIR, TGA and DSC analyses. Thermal analyses demonstrated that T<sub>g</sub> of PLA shifted to higher temperatures in parallel with crosslinking density at the polymer-ceramic interface. In addition, Vicker's hardness tests were performed to reveal the effect of silane modifying agents on hardness before and after the in vitro degradation test. PLA/F-HAp showed a lesser weight loss after in vitro degradation test as well as an increased Vicker's Hardness compared to the reference (unmodified PLA/HAp) system. Findings demonstrated that increased crosslinking density between PLA and HAp interface not only enhanced the degradation profile of PLA matrix it also improved the mechanical behavior of the structure.

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# Keywords

Biomaterials Biocomposites PLA/HAp composites Surface modification

### Last published paper details

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### Full title of article

Monitoring of Thiamethoxam Resistance in Turkish House Fly Strains, Musca domestica (Diptera: Muscidae)

### Journal

Journal of Arthropod-Borne Diseases

### Year

2024

### Volume

17

### First page

206-213

# All authors

Huseyin Cetin, Atila Yanikoglu, Esin Akarsu, Mehmet Civril, Eylul Odabas, Samed Koc, Emre Oz, Burak Polat

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# Abstract

Hydrogen sulfide ( $H_2S$ ) is a toxic gas which is highly flammable and falls under the category of chemical asphyxiant, along with carbon monoxide and cyanide gases. Although  $H_2S$  has characteristic odor of rotten egg however, at high concentrations above 100ppm, the olfactory nerves can become temporarily paralyzed due to saturation, compromising the sense of smell. Colorimetric method is the most used approach for the detection of  $H_2S$ . Commercial lead acetate-based paper strips are available which can qualitatively detect  $H_2S$  by changing its color from white to black when exposed to  $H_2S$ . Although the lead acetate-based paper strip is inexpensive, its use is limited due to low sensitivity and the toxicity of metallic lead. More recently photothermal approach has been reported for the detection of  $H_2S$ . Photothermal materials have received a great deal of attention in recent years owing to their unique light-to-heat photo-physical conversion property which can be exploited for detection of different analytes. Photothermal sensing of the analytes is exceptionally promising for onsite analysis. The interaction of the analyte alters the photothermal response of the sensing material, which can be measured by a thermometer or a photothermal camera. These devices are portable, inexpensive, and widely available.

Here we have prepared copper acetate-based inkjet-printable inks with excellent printability. In this study, we present an easy-to-use cheap spoilage sensor for food packaging. The sensor is based on H<sub>2</sub>S-detection and can be read either by simple colorimetric or photothermal response.

The sensing films are characterized by X-ray photoelectron spectroscopy (XPS). The photothermal response has been measured with FLIR E8 Thermal Imaging Camera. The change in colour of the exposed sensors was evaluated by CIELab color space.

# Keywords

Spoilage Sensor Photothermal X-ray photoelectron spectroscopy

# Last published paper details

These are the highlights from our last paper: An approach to fabricate a low-cost, mass producible, flexible, and disposable SERS-active substrate is reported. The nanostructured substrates are produced by roll-to-roll coating a two-component latex dispersion onto paperboard. The SERS functionality is obtained by physical vapor deposition of an ultra-thin layer of Au or Ag (2.5-5 nm). The surface nanostructure was confirmed by atomic force microscopy. The SERS effect was confirmed by two model compounds; crystal violet and rhodamine 6G.

# Full title of article

Low-cost, mass-producible nanostructured surface on flexible substrate with ultra-thin gold or silver film for SERS applications

# Journal

Nano-Structures & Nano-Objects

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All authors

Emil Rosqvist, Ulrike Böcker, Tina Gulin-Sarfraz, Nils Kristian Afseth, Stiina Tolvanen, Jouko Peltonen, Jawad Sarfraz

# DOI

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# P.145 Evaluation of interfacial interactions between polymer coating and ion-substituted ceramic scaffolds

<u>Yaşar Murat Elçin</u>, Seyithan Kansız, Murat Taner Vurat, Mahmut Parmaksiz, Ayşe Eser Elçin Tissue Engineering, Biomaterials and Nanobiotechnology Laboratory, Ankara University Faculty of Science & Ankara University Stem Cell Institute, Ankara, Turkey

# Abstract

Hydroxyapatite (HAp) is a calcium phosphate-based bioactive ceramic widely used in hard tissue repair applications. Recently, the use of dopants such as sodium (Na<sup>+</sup>), magnesium (Mg<sup>2+</sup>), zinc (Zn<sup>2+</sup>), copper (Cu<sup>2+</sup>), silica (SiO<sub>4</sub><sup>-</sup>), strontium (Sr<sup>2+</sup>) and boron (BO<sub>3</sub><sup>-</sup>) has become an attractive approach in order to increase the osteogenic properties of HAp.

In bone tissue, strontium is present in low concentrations between 0.008 and 0.010%. Studies have shown that  $Sr^{2+}$  ions play a key role in the maturation of osteoblasts into osteocytes and in the bone regeneration process. Therefore,  $Sr^{2+}$  doped HAp particles are widely used in hard tissue applications to enhance cell proliferation and bone growth. Boron is another trace element found in the structure of bone. In in vitro studies, boron was found to increase collagen type I, osteopontin, bone sialoprotein and osteocalcin gene expression. It has also been reported that boron supplementation increases cortical and trabecular bone volume fractions in mice.

In this study, HAp particles having different dopants, including boron doped (B-HAp), strontium doped (Sr-HAp) and both boron and strontium doped (B-Sr-HAp) particles, were synthesized to prepare ceramic scaffolds using the sponge replica method. Polyvinyl alcohol and chitosan (PVA/Chi) were coated to the surface of ceramic scaffolds to investigate the effect of surface properties on the coating of PVA/Chi. The prepared biocomposites were characterized using SEM, FTIR, TGA, and DSC analyses to demonstrate the effect of surface chemistry on PVA/Chi coating. The findings showed that HAp could only form hydrogen bonds with PVA/Chi, while the coating efficiency of B-HAp and Sr-HAp was directly affected by ionic interactions and borate-diol complexation reactions, respectively. The most striking result was obtained for B-Sr-HAp, which has both ionic interactions and borate-diol complexation reaction at the polymer-ceramic interface.

# Keywords

Biocomposite Ion-Doped Hydroxyapatite PVA/Chitosan coating Interface Interaction

# Last published paper details

Adv Colloid Interface Sci . 2023 Jul:317:102930. doi: 10.1016/j.cis.2023.102930.

# Full title of article

Advanced liposome and polymersome-based drug delivery systems: Considerations for physicochemical properties, targeting strategies and stimuli-sensitive approaches

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Advances in Colloid and Interface Science

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# P.146 Antiviral and antibacterial cotton fabric functionalized with ZnONPs/CuNPs and silane

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# Abstract

The COVID-19 pandemic has emphasized the vital importance of bioactive textile materials, drawing attention to their significance in a tragic way. This has underscored the need for continued research and development in this area to enhance public health and safety.

The application of zinc oxide (ZnONPs) or copper (CuNPs) nanoparticles to cellulose fabric has documented potential as antimicrobial modifiers [1–2]. To provide the best protection against viruses, it is essential to use textile materials with antiviral, antibacterial, and non-toxic properties. To serve this purpose, we have developed a modified cotton fabric (CO) by incorporating 1 wt.% and 2.5 wt.% of ZnONPs and CuNPs, as well as a mixture of both, along with vinyltrimethoxysilane (VIN).

To characterize the physic-chemical effects of the fabric modification the SEM/EDS and AAS analysis, Raman and FTIR spectroscopy and goniometric analysis were used.

All modified fabrics have good and very good antiviral activity against human coronavirus HCoV 229E and are non-toxic against non-tumorigenic, immortalized human keratinocyte cells HaCat and human lung adenocarcinoma cells A549.

# They have strong antibacterial activity against Gram-negative (*Klebsiella pneumoniae*) and Gram-positive (*Staphylococcus aureus*) bacteria.

After application of CuNPs and ZnONPs the water contact angle values amount about 140 degree for all modified fabrics, which are hydrophobic. The surface free energy values decreased from 30 mJ/m<sup>2</sup> for unmodified CO fabric to 11 mJ/m<sup>2</sup> for all fabrics with 1 wt.% of nanoparticles and to 23 mJ/m<sup>2</sup>, 14 mJ/m<sup>2</sup> and 16 mJ/m<sup>2</sup> for fabrics with 2.5 wt.% of CuNPs, ZnONPs and their mixture, respectively.

# References

- [1] M. Cieślak et al., Materials, 15 (2022) 1–16.
- [2] M. Cieślak et al., Cellulose, 30 (2023) 9843–9859.

# Acknowledgment

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# Keywords

cotton fabric zinc oxide and copper nanoparticles antiviral and antibacterial properties goniometric analysis

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# Full title of article

AgNWs-Silane Coatings for the Functionalization of Aramid Woven Fabrics

# Journal

Coatings

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# All authors

Alicja Nejman, Anna Baranowska-Korczyc, Grzegorz Celichowski, Małgorzata Cieślak

DOI

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# P.147 Pressure-adhesive patches loaded with Quercus infectoria extract as antimicrobial wound dressings for chronic infections

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# Abstract

Chronic wound infections that cause delayed healing are an enormous challenge. Traditional wound treatments such as gauze have poor antibacterial properties and may adhere to the wound bed and disrupt wound healing. Novel active pressure-sensitive adhesive patches from natural rubber incorporating *Quercus infectoria* (*Qi*) with prolonged release was developed as an efficient antimicrobial wound dressing for chronic wound treatment. Physical characterization demonstrated that *Qi*-loaded patches exhibited hydrophilicity properties with contact angle of 64.94°. Thermal stability of the adhesive patches determining by thermogravimetric analysis was observed at 200 °C. The peel strength and shear strength of the *Qi*-loaded patches were significantly increased as 3.80 ×  $10^2$  N/m and  $6.59 \times 10^4$  N/m<sup>2</sup>, respectively, compared with unloaded patches (*p* < 0.05). The dry patches could also absorb up to 700-fold its weight in wound fluid, effectively providing a moist wound environment and allowing for gas exchanges. When tested against

reference strains and clinical isolates, including Gram-positive, Gram-negative bacteria and fungi, the *Qi*-loaded patches showed significant reductions compared with the blank patch (p < 0.05). In addition, the *Qi*-loaded patches showed significantly higher scavenging activities against DPPH and ABTS radicals with a value of more than 90% and 100%, respectively (p < 0.05). FRAP assay demonstrated a ferric ion reducing power in a concentration-dependent manner. Fourier-transform infrared spectroscopy indicated that the formulation did not interact chemically with pressure-sensitive adhesive patches. The *in vitro* release of gallic acid from *Qi*-loaded patches, as standard marker is fitted to Higuchi's model in which the active compound can diffuse from the matrix patches. A safety evaluation of the patch proved cell viability of 99% and non-cytotoxicity in direct contact with L929 fibroblast cells. In addition, *Qi*-loaded patches. The findings indicated that *Qi*-loaded patches caused rapid blood clotting within 10 min when compared with unloaded patches. The findings indicated that *Qi*-loaded patches could be a good candidate for wound dressing due to their promising physical and biological properties.

# Keywords

natural rubber pressure-sensitive adhesive Quercus infectoria wound dressings

### Last published paper details

Tassanai Waen-ngoen, Suttiwan Wunnoo, Ozioma Forstinus Nwabor, Siwaporn Bilhman, Krittima Dumjun, Jomkwan Ongarj, Nawamin Pinpathomrat, Sakkarin Lethongkam, Supayang Piyawan Voravuthikunchai, Supakit Paosen, Effectiveness of plant-based hand sanitizer incorporating Quercus infectoria gall extract, Journal of Applied Microbiology, Volume 134, Issue 12, December 2023, Ixad295, https://doi.org/10.1093/jambio/Ixad295

## Full title of article

Effectiveness of plant-based hand sanitizer incorporating Quercus infectoria gall extract

### Journal

Journal of Applied Microbiology

Year

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### Volume

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# All authors

Tassanai Waen-ngoen, Suttiwan Wunnoo, Ozioma Forstinus Nwabor, Siwaporn Bilhman, Krittima Dumjun, Jomkwan Ongarj, Nawamin Pinpathomrat, Sakkarin Lethongkam, Supayang Piyawan Voravuthikunchai, Supakit Paosen

# DOI

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# P.148 Development of natural extract-loaded hydrogels containing *Quercus infectoria*encapsulated chitosan nanoparticles for the prevention of bovine mastitis

Supakit Paosen<sup>1</sup>, Sireetorn Kurakaeo<sup>1</sup>, Paramee Isaro<sup>2</sup>, Kanyapak Petnoo<sup>2</sup>, Supayang P. Voravuthikunchai<sup>1</sup>, <u>Sakkarin</u> Lethongkam<sup>1</sup>

<sup>1</sup>Prince of Songkla University Faculty of Science, Thailand. <sup>2</sup>PSU.Wittayanusorn School, Thailand

# Abstract

Nanoencapsulation technology is attracting interest in drug delivery systems as unstable bioactive compounds are protected from undesired environments. It has been used in several applications including agricultural purposes. Bovine mastitis is one of the most problematic infectious diseases in dairy cattle. It is the main cause of economic losses due to reduced milk production and poor-guality milk. Using antibiotics or antiseptics for the prevention and treatment of the disease can lead to the development of multidrug-resistant pathogens. The current study aims to develop a novel biocompatible hydrogel loaded with a combination of Quercus infectoria gall, Rhodomyrtus tomentosa leaf extracts, and Q. infectoria encapsulated chitosan nanoparticles (Qi nano). Microorganisms were first isolated from bovine teats and raw milk and then identified bacterial species using MALDI-TOF mass spectrometry. Staphylococcus chromogenes was selected as a representative of Gram-positive bacteria while Pseudomonas sp. and Acinetobacter sp. were selected as representative Gram-negative bacteria. Qi nano was successfully synthesized using an ionic gelation method with sizes of approximately 150-200 nm. Carboxymethyl cellulose-based hydrogel was mixed with the extracts and the nanoparticles, and biological efficacies of the hydrogel were further evaluated. The hydrogel exhibited strong antioxidant and antibacterial activity with minimum inhibitory concentration and minimum bactericidal concentration against isolated bacteria ranging between 3.90-31.25 mg/mL and 15.62-250 mg/mL, respectively. A significant reduction of biofilm formation was demonstrated, compared with untreated control (p < 0.05). The natural extract incorporated-hydrogel showed antiinflammatory activity by inhibiting nitric oxide production of lipopolysaccharide-simulated raw 264.7 cells. Moreover, approximately 99.9% of the tested bacteria were inhibited by the hydrogel in an ex vivo infection model. The promising results presented in this study are suggesting that the novel biocompatible natural product-loaded hydrogel is a potent alternative for the control of bovine mastitis in dairy cattle.

# Keywords

Quercus infectoria chitosan nanoparticles mastitis hydrogel

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Lethongkam S, Glaser J, Ammanath AV, Voravuthikunchai SP, Götz F. In vitro and in vivo comparative analysis of antibacterial activity of green-synthesized silver nanoparticles. Biotechnology Journal 2023, 2300186.

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In vitro and in vivo comparative analysis of antibacterial activity of green-synthesized silver nanoparticles

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All authors

# DOI

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# P.149 Separation and encapsulation of mRNA for vaccine and therapeutic applications

<u>Ehsan Nourafkan</u>, Zidi Yang, Charlotte Kenyon, Adithya Nair, Kate A Loveday, Emma N Welbourne, Mahdi Ahmed, Joseph Middleton, Mark J Dickman, Solomon F Brown, Mabrouka Maamra, Joan Cordiner, Zoltan Kis University of Sheffield, UK

# Abstract

After the COVID-19 pandemic, several companies and organizations are actively developing, scaling up and optimizing mRNA manufacturing processes to produce their vaccines and therapeutics. Our work delves into the methodologies for effectively separating, concentrating and encapsulation of mRNA drug substance. For the first time, the membrane fouling behavior caused by mRNA and the separation of nucleoside triphosphates (NTPs) was mathematically modelled. The mRNA membrane fouling model is necessary for optimizing the mRNA separation process, designing a suitable strategy for membrane clean up, estimating the end of production life and reduction of the process cost. mRNA recovery greater than 70% without degradation after the filtration and mRNA encapsulation efficiency higher than 90% were obtained.

## Keywords

mRNA separation mRNA encapsulation Membrane fouling Lipid nanoparticles

### Last published paper details

https://pubs.rsc.org/en/content/articlelanding/2022/sm/d1sm01326b#!

## Full title of article

Minimum surfactant concentration required for inducing self-shaping of oil droplets and competitive adsorption effects

### Journal

Soft matters

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### All authors

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# P.150 Affordable polymer grafting for sustainable high-performance carbon electrode-based perovskite solar cells

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# Abstract

Carbon electrode-based perovskite solar cells (C-PSCs) are known for their cost-effective manufacturing process and long-term stability. However, their performance and durability have been limited by poor contact between the hole transporting layer (HTL) and the carbon electrode. This study presents an innovative approach to enhance C-PSC performance. A low-cost polymer is synthesized under ambient air conditions with moderate humidity (35-45% RH). To boost device performance, an ultrathin layer of polyethylene glycol (PEG, 20000 MW) is applied for surface passivation between the copper(I) thiocyanate (CuSCN) HTL and the carbon electrode. This passivation technique significantly increases the power conversion efficiency (PCE) from 12.52% (untreated) to 15.66%, surpassing the performance of conventional doped spiro-OMeTAD-based devices (14.48%). The results demonstrate that PEG not only forms a self-repairing layer and reduces interface issues but also optimizes energy band alignment between the HTL and the carbon electrode, facilitating more efficient charge transfer. Moreover, PEG grafting provides moisture protection, enhancing the device's thermal stability. PEG-treated C-PSCs exhibit superior long-term stability (>90% for 1000 hours) in ambient air and thermal stability after aging at 85 °C, 80-90% RH (>80% for 1000 mins) without encapsulation. Furthermore, these devices demonstrate excellent performance for indoor applications under LED 1000 lux illuminations, achieving PCEs of 36.29% and 35.38% with active areas of 0.09 and 1.00 cm<sup>2</sup>, respectively. These findings provide a basis for the development of cost-effective, stable, and scalable C-PSCs suitable for indoor applications and nondestructive encapsulation, offering a promising pathway for future commercialization.



# Keywords

Carbon-based perovskite solar cells Polyethylene glycol Sustainability

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# Surface passivation

## Last published paper details

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## Full title of article

A novel carbon electrode for up-scaling flexible perovskite solar cells

## Journal

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101895

# All authors

Woraprom Passatorntaschakorn, Warunee Khampa, Wongsathon Musikpan, Chawalit Bhoomanee, Athipong Ngamjarurojana, Sakhorn Rimjaem, Atcharawon Gardchareon, Chatchai Rodwihok, Han S. Kim, Nutcha Khambunkoed, Ratchadaporn Supruangnet, Hideki Nakajima, Ladda Srathongsian, Pongsakorn Kanjanaboos, Akarin Intaniwet, Anusit Kaewprajak, Pisist Kumnorkaew, Fabrice Goubard, Pipat Ruankham, Duangmanee Wongratanaphisan

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# P.151 A dual approach of additive engineering and surface passivation with TiO<sub>2</sub>-TiAcAc/SnO<sub>2</sub> electron transporting layer in carbon-based perovskite solar cells

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# Abstract

Efficient electron transport layers (ETLs) are essential for the successful operation of highefficiency carbon-based perovskite solar cells (C-PSCs). However, widely used metal oxide electron transport layers (ETLs) such as TiO<sub>2</sub> often confront challenges such as low electrical conductivity and high surface defect density. This work proposes an approach to address the challenge by employing a dual strategy involving additive engineering and surface passivation with a TiO<sub>2</sub>-TiAcAc/SnO<sub>2</sub> electron transporting layer through a low-temperature procedure ( $\leq$ 150°C). In the additive engineering approach, a solution of TiO<sub>2</sub> nanoparticles (TiO<sub>2</sub> NPs) is merged with titanium diisopropoxide bis(acetylacetonate) (TiAcAc) to produce TiO<sub>2</sub>-TiAcAc ETL. This results in the formation of uniform and well-adhered TiO<sub>2</sub> film, which substantially increases the open-circuit voltage (V<sub>OC</sub>) to 1.10V. Furthermore, the TiO<sub>2</sub>-TiAcAc ETL is treated with an ultrathin layer of SnO<sub>2</sub>, resulting in an enhancement of the fill factor (FF). By employing this surface passivation approach, surface and interface defects of TiO<sub>2</sub>-TiAcAc ETL could be diminished. Consequently, C-PSCs with an active area of 0.09 cm<sup>2</sup>, utilizing a TiO<sub>2</sub>-TiAcAc/SnO<sub>2</sub> ETL and fabricated under dry air environment, achieves a maximum PCE of 16.00% with an open-circuit voltage (V<sub>OC</sub>) of 1.09V, a short-circuit current density (J<sub>SC</sub>) of 20.34 mA cm<sup>-2</sup>, and a fill factor (FF) of 72.00%. This work demonstrates the effectiveness of a dual approach in significantly boosting the photovoltaic performance of C-PSCs, paving the way for their future advancements.



# Keywords

Carbon-based perovskite solar cells Electron transporting layer Additive engineering Surface passivation

### Last published paper details

Khampa, W., Bhoomanee, C., Musikpan, W., Passatorntaschakorn, W., Rodwihok, C., Kim, H. S., Gardchareon, A., Ruankham, P., & Wongratanaphisan, D. (2023). A passivation by H2O2-TiO2 interlayer for efficient and stable carbonbased perovskite solar cells. Applied Surface Science, 637, 157933.

### Full title of article

A passivation by H2O2-TiO2 interlayer for efficient and stable carbon-based perovskite solar cells

### Journal

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### Year

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# All authors

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# DOI

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# P.152 Manufacturing of solid oxide fuel cells: Novel ceramic processes

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<sup>1</sup>Resoh Solutions SRL, Italy. <sup>2</sup>Dipartimento di Ingegneria "Enzo Ferrari", Università degli studi di Modena e Reggio Emilia, Italy. <sup>3</sup>Department of Industrial Engineering, University of Florence, Italy. <sup>4</sup>National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy

# Abstract

This study explores the manufacturing of solid oxide cells (SOCs) and introduces innovative ceramic processes essential to their production. The research primarily focuses on the manufacturing and characterization of porous supports manufactured from yttria-stabilized zirconia (3YSZ). The methodology involves a pioneering technique employing digital deposition of dry powders and ink-jet printing followed by pressing.

Solid oxide cells (SOCs) stand as advanced ceramic devices employed in diverse electrochemical applications, including solid oxide fuel cells (SOFCs) and solid oxide electrolysis cells (SOECs). SOFCs exhibit distinct advantages over alternative fuel cell types, boasting high efficiency, fuel adaptability, and minimal emissions. They demonstrate the capability to operate with various fuels, including hydrogen, natural gas, and biogas, suggesting their potential to supersede traditional power generation technologies due to heightened efficiency and reduced environmental impact. Notably, these cells are reversible and can facilitate hydrogen gas production through steam electrolysis (SOEC).

This research focuses on formulating and testing diverse compositions of porous supports, incorporating distinct types, shapes, and sizes of pore formers. Strength and stiffness properties of the sintered bodies are assessed using advanced techniques, encompassing scanning electron microscopy, mercury porosimetry, ultrasound methodologies for determining Young's modulus, and measuring mechanical bending strength.

Results elucidate a clear correlation between increased total porosity and an exponential decrease in Young's modulus and strength. Meticulously manufactured and characterized 3YSZ samples undergo comprehensive analysis to evaluate their suitability as support structures in solid oxide electrolysis or fuel cell applications. The findings from this research offer invaluable insights for designing and developing porous materials utilizing the proposed innovative processes, with the potential to enhance the production of cells for state-of-the-art electrochemical technologies.

### Keywords

solid oxide cells ink-jet printing hydrogen porous supports

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### Full title of article

Preliminary study on the design of superhydrophobic surface by 3D inkjet printing of a sol-gel solution

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Journal of Sol-Gel Science and Technology

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Volume

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368

# All authors

Rosa Taurino, Maria Cannio, Dino Norberto Boccaccini, Massimo Messori, Federica Bondioli

# P.153 Functionalized non-woven structure with antimicrobial activity

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<sup>1</sup>Lukasiewicz Research Network- Lodz Institute of Technology, Department of Chemical Textile Technology, Marii Sklodowskiej–Curie, Lodz, Poland. <sup>2</sup>Department of Nanobiology and Biomaterials, Military Institute of Hygiene and Epidemiology, Kozielska, Warsaw, Poland

## Abstract

The textile sector demands continuous innovation to develop new solutions that can customize fabrics with specific properties according to their intended use. The coronavirus epidemic caused a particular increase in interest in developing a textile with antiviral properties [1,2].

In order to obtain such properties, various materials and modification methods were tested. Developing a textile with antiviral properties is a complex process. It involves considering the structure and composition of the textile, selecting bioactive modifiers, and using effective application methods. Nonwoven structures offer great potential for use in filtration, protective systems, and covering materials.

We have designed a non-woven structure that combines hydrophobic (polyester) and hydrophilic (viscose) fibers, two nanomodifiers (2.5% of ZnO or/and Cu) and vinyltrimethoxysilane (VIN), which is specifically tailored to the structure and adsorption mechanism of the human coronavirus.

The modification effects were characterized using SEM/EDS and AAS analysis, along with Raman and FTIR spectroscopy. The surface and thermal properties were investigated using respectively, goniometric and DSC and TG/DTG techniques.

The antibacterial activity was assessed against both Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Klebsiella pneumoniae*) bacteria, while the antiviral properties were tested against the HCoV 229E human coronavirus, a known pathogen causing upper respiratory tract diseases.

The functional non-woven fabrics we have obtained exhibit antiviral properties and are non-toxic to non-tumorigenic, immortalized human keratinocyte cells (HaCat) and human lung adenocarcinoma cells (A549).

[1] Y. Oguz-Gouillart et al., Advanced and Smart Textiles during and after the COVID-19 Pandemic: Issues, Challenges, and Innovations, *Healthc.*, 11(8), 2023, doi: 10.3390/healthcare11081115.

[2] M. Cieślak et al, Effect of Cu Modified Textile Structures on Antibacterial and Antiviral Protection, *Materials*, 15(17), 1–16, 2022, doi: 10.3390/ma15176164.

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# Keywords

antimicrobal textiles anti-viral non-woven coronavirus nanomodifiers

# Last published paper details

O. Frączak et al., "Raman spectroscopy and gas chromatography with flame ionization detection as analysis tools in stability tests of selected synthetic psychoactive substances: 5-IT, MT-45 and 4-CMC," Vib. Spectrosc., vol. 111, 2020, doi: 10.1016/j.vibspec.2020.103176.

## Full title of article

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Vibrational Spectroscopy

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2020

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111

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103176

# All authors

Oliwia Frączak , Kinga Kądzioła-Długołęcka , Ilona Kijewska, Radosław Wilczek , Beata Tkacz-Szczęsna , Krzysztof Makowski , Piotr Komorowski, Robert Bachliński , Anna Trynda , Bogdan Walkowiak

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# P.154 Non-Ti MXene as an electrode materials for supercapacitors

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# Abstract

MXene is one of the most interesting two-dimensional (2D) materials that have been discovered. With more than 70% of publication-related studies, titanium-based MXene (Ti-MXene) has been well-evaluated, hence, laying the very first foundation of the 2D MXene with tailorable properties acquainted with a diverse range of applications. Yet there are still other candidates amongst transitional metals that can play the role of 2D MXene well beyond known applications. Herein, we have reported free-standing and binder-free non-Ti MXene as an active electrode as a supercapacitor electrode material. The free-standing non-Ti MXene film is based on a colloidal solution. The electrode exhibited excellent electrochemical performance in various electrolytes. This study not only elucidates the charge storage process of non-Ti MXenes but also provides new insights for designing novel electrode materials for energy storage devices.

# Keywords

MXene electrode supercapacitor

# Last published paper details

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# Full title of article

MXene-based heterostructures: Current trend and development in electrochemical energy storage devices

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101097

## All authors

Iftikhar Hussain, Charmaine Lamiel, Muhammad Sufyan Javed, Muhammad Ahmad, Sumanta Sahoo e, Xi Chen a, Ning Qin, Sarmad Iqbal, Shuai Gu, Yuxiang Li, Christodoulos Chatzichristodoulou, Kaili Zhang

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# P.155 Design and characterization of based chitosan sol-gel films for textile substrates: Traditional and 3D printing processes approach

<u>Rosa Taurino</u><sup>1,2</sup>, Maria Cannio<sup>3</sup>, Stefano Caporali<sup>1,2</sup>, Stefano Martinuzzi<sup>1,2</sup>, Dino Boccaccini<sup>3</sup> <sup>1</sup>Department of Industrial Engineering, University of Florence,, Italy. <sup>2</sup>National Interuniversity Consortium of Materials Science and Technology (INSTM), Italy. <sup>3</sup>Resoh Solutions S.r.I., Italy

## Abstract

This research aimed to develop an innovative textile finish using chitosan sol-gel coatings to imbue fabrics with selfcleaning properties, ultraviolet (UV) protection, wear resistance, and oil repellency.

Chitosan, a bioactive polymer renowned for its antibacterial activity, non-toxicity, ease of modification, and biodegradability, serves as a promising candidate for multifunctional coatings, as evidenced by extensive scientific literature. Within the context of environmental sustainability, chitosan-based organic-inorganic hybrid coatings offer significant potential for the creation of advanced protective layers. In this investigation, organic-inorganic hybrid coatings were synthesized using tetraethyl orthosilicate (TEOS) as the inorganic silica network precursor and chitosan as the organic component. To optimize adhesive strength and water resistance, two different coupling agents, vinyltrimethoxysilane (VTMS) and 3glycidyloxypropyl)trimethoxysilane(GLYMO), were employed and compared. Various formulation of sol-gel hybrids loaded with different amounts of chitosan were prepared and applied onto different textile substrates (cotton and synthetic filter fabrics) by airbrushing technique. Furthermore, recognizing the remarkable versatility demonstrated by the inkjet printing process, we optimized the sol-gel solution composition for digital injection techniques. Our findings unequivocally demonstrate that chitosan concentration and the type of coupling agent wield significant influence over jetting stability. Moreover, we conducted a comprehensive analysis of the effect of film composition on several properties through Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) for microstructure examination, water contact angle measurements for surface wettability assessment, hydrolitic degradation tests, and mechanical characterization. These investigations shed light on the intricate interplay between film composition and material properties, providing valuable insights for the development of advanced textile finishes.

### Keywords

sol-gel process chitosan 3D printing textile

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### Full title of article

Preliminary study on the design of superhydrophobic surface by 3D inkjet printing of a sol-gel solution

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368

# All authors

R. Taurino, M. Cannio, D.N. Boccaccini, M. Messori, F. Bondioli

# **P.156** Towards the development of fast, yet accurate, simulations of surfactant systems: The role of local density dependent potentials

<u>James O'Connor</u><sup>1</sup>, Joanne Cook<sup>2</sup>, Ian Stott<sup>2</sup>, Andrew Masters<sup>1</sup>, Carlos Avendaño<sup>1</sup> <sup>1</sup>The University of Manchester, UK. <sup>2</sup>Unilever R&D Port Sunlight, UK

# Abstract

The Holy Grail for the simulation of surfactant systems is a methodology that combines high computational efficiency with the accurate prediction of thermophysical properties. Coarse-grained methodologies, such as Dissipative Particle Dynamics, use ultra-soft interaction potentials to achieve the efficiency goal, but these gains commonly come at the expense of the accuracy of property prediction. On the other hand, molecular-based equations of state, such as the Statistical Associating Fluid Theory (SAFT), provide accurate descriptions of the thermodynamics of complex fluids but cannot be used to study the inhomogeneous phases typically found in surfactant systems.

A promising way forward is to make use of local density dependent potentials, where the potential is derived from an underlying, accurate equation of state. The softness of the potential allows for high computational speed while the underlying equation of state provides highly accurate property prediction. To achieve this aim for surfactant systems, one needs to build up the model step by step. Fundamental requirements are good models for water, for alkanes and for the alkane-water interface.

Here we describe the development of such a model *via* the use of local density dependent potentials based on the SAFTg-Mie equation of state. We demonstrate that our methodology provides accurate predictions for the thermodynamic properties of water over a wide range of temperatures. These include both the vapour-liquid co-existence curve and the surface tension of the water/vapour interface. A similar methodology is also shown to work well for the bulk and surface properties of a variety of alkanes. Preliminary results will be provided for water/alkane mixtures.

We believe that this work provides a sound basis for the development of simulation models that can tackle the complex soft matter phases exhibited by surfactant systems, combining both speed and accuracy.

# Keywords

Water Surfactants Oil Mesoscale Simulation

### Last published paper details

James P. D. O'Connor, Joanne L. Cook, Ian P. Stott, Andrew J. Masters, Carlos Avendaño; Local density dependent potentials for an underlying van der Waals equation of state: A simulation and density functional theory analysis. J. Chem. Phys. 21 November 2023; 159 (19): 194109

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# All authors

J. P. D. O'Connor, J. L. Cook, I. P. Stott, A. J. Masters, C. Avendaño

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# P.157 Synthesis, characterization and properties of acrylic core-shell latexes: Effect of poly(styrene-co-acrylonitrile) as hard-core

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# Abstract

The potential enhancement of polymer matrix properties through the addition of dispersed material has been widely demonstrated. In the pursuit of exploring this, we carried out the synthesis of a core-shell latex via semi-batch emulsion polymerization. The hard-core was composed of poly(styrene-*co*-acrylonitrile) (SAN), while the soft-shell consisted of poly(butyl acrylate-*co*-styrene-*co*-acrylamide) (BASAAD). The high difference between glass transition temperature ( $T_g$ ) of such polymers provided versatility in processing since it allowed us to cast a blend material from the latex at moderate temperatures.

The resulting latex particles and casted polymers were characterized by using electron microscopy in order to show the differences in morphology depending of core composition. Given SAN's recognized mechanical, thermal, and barrier properties, we also studied the effect of having nano-sized dispersed SAN polymer into a soft acrylic matrix. Furthermore, we systematically varied SAN composition and core-shell weight ratio to comprehensively evaluate their influence on the properties of the final latex and polymer blend.

These waterborne acrylic core-shell latexes have been designed to be applied as promising coatings aimed to address the multifaceted demands of the packaging market.



# Keywords

emulsion polymerization latex coatings SAN

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All authors

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P.158 Oil and particle interaction in porous structures

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## Abstract

Soil matrix has porous structures assembled by solid parts and confined pores located between them. Oil residues from petroleum pollutants and hydrophobic pesticides can exist as small droplets even after chemical remediation. When exposed to solid particles like microplastic or mineral particles, oil droplets may form Pickering emulsions which are rather stable and tend to clog the intrinsic pore throats. As a result, the permeability of soil matrix may be reduced and the flow properties may be changed. This can affect the efficiency of soil remediation methods, e.g. phytoremediation, bioventing. Understanding the interactions between oil and particles is critically important for selecting an appropriate method for the effective cleanup of a contaminated site.

We study the interactions between model oil droplets and calcium carbonate microparticles in bulk solutions with TurbiScan by measuring the transmission and backscattering light intensity of an incident light. Creaming, sedimentation and coalescence dynamics are analyzed. Different emulsion types are formed with an increasing concentration of CaCO<sub>3</sub>. At lower concentration (0.1 wt%), oil droplets in water are formed after mixing, while they coalesce into larger drops and eventually separate into layers. The particles accumulate on the oil-water interface. At higher concentrations (5 wt% and 10 wt%), water-in-oil emulsions are formed, where only creaming is observed. Salt added to the water phase increases the affinity of the oil phase to the glass vessel wall. Increasing NaCl concentration would induce aggregation of CaCO<sub>3</sub> particles. Their interactions are further studied in 1D confined pores with microfluidic droplet generation, where oil droplets are generated in particle solutions (0.1 wt%). Solid particles are found to accumulate on the oil-water interface, enhancing the affinity between droplets and the channel walls. Oil droplets coalesce into larger ones or aggregate into clusters that would clog the microfluidic channel. The microfluidic results are in agreement with bulk behaviors.

## Keywords

Particle Oil Porous structure Soil remediation

### Last published paper details

Tian Wang, Simon Ivar Andersen, Alexander Shapiro. Coalescence of oil droplets in microchannels under brine flow. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2020, 598, 124864.

### Full title of article

Coalescence of oil droplets in microchannels under brine flow

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### All authors

T. Wang, S. I. Andersen, A. Shapiro

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# P.159 Development of c-phycocyanin/whey protein isolate-zein nanoparticles by pH-shifting method

Moises Job Galindo-Pérez<sup>1</sup>, Lizbeth Martínez-Acevedo<sup>2</sup>, Dolores Reyes-Duarte<sup>1</sup>, Marcia Morales-Ibarría<sup>1</sup>, Izlia Jazheel Arroyo-Maya<sup>1</sup>, José Campos-Terán<sup>1</sup>

<sup>1</sup>Universidad Autónoma Metropolitana-Cuajimalpa, Mexico. <sup>2</sup>Universidad Autónoma Metropolitana-Xochimilco, Mexico

# Abstract

The proteins derived from cyanobacteria, such as C-phycocyanin (C-PC), have gained interest in the food industry due to their functional properties. One characteristic of C-PC is its bright blue color, making it useful as a natural food colorant. However, C-PC can undergo degradation due to various physicochemical factors, limiting its applications. An alternative for its stabilization is nanoencapsulation. Therefore, this work aimed to determine the optimal conditions for preparing C-PC nanoparticles using whey protein isolate (WPI) and zein as proteins for self-assembly through the electrostatic interaction by pH-shifting method. A 2<sup>3</sup>-factorial design was conducted, where the independent variables were the zein (1 to 10 mg/mL), WPI (1 to 10 mg/mL), and C-PC (0.5 to 1.5 mg/mL). The response variables included particle size (PS), polydispersity index (PDI), zeta potential ( $\zeta$ ), encapsulation efficiency (EE), and process efficiency (PE). According to the desirability analysis (D=0.757), the optimal conditions for obtaining nanoparticles were found. Under these conditions, nanoparticles with PS of around 203.34 ± 8.37 nm, PDI of 0.253 ± 0.01,  $\zeta$ of -16.20  $\pm$  1.63 mV, EE of 68  $\pm$  7.54%, and PE of 96.7  $\pm$  1.2% were obtained. The polyhedral morphology of the nanoparticles was evidenced through scanning electron microscopy (SEM). The nanoparticles maintained their physicochemical properties for 90 days in refrigerated storage, preserving the C-PC amount. With the factorial design and the green methodology of pH-shifting self-assembly, the conditions to prepare the C-PC/WPI-zein nanoparticles were established, with potential applications in food and pharmaceutical areas.

# Keywords

c-phycocyanin zein nanoparticles food materials

# Last published paper details

"Electrostatic interactions control the adsorption of extracellular vesicles onto supported lipid bilayers" Andrea Ridolfia, Jacopo Cardellinib, Fatlinda Gashi, Martijn J.C. van Herwijnen, Martin Trulsson, José Campos-Terán, Marca H. M. Wauben, Debora Berti, Tommy Nylander, Joakim Stenhammar Journal of Colloid and Interface Science (2023), 65 (A), 883-891 Published: 15 November 2023 https://doi.org/10.1016/j.jcis.2023.07.018

# Full title of article

Electrostatic interactions control the adsorption of extracellular vesicles onto supported lipid bilayers

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## First page

883

## All authors

Andrea Ridolfi, Jacopo Cardellini, Fatlinda Gashi, Martijn J.C. van Herwijnen, Martin Trulsson, José Campos-Terán, Marca H. M. Wauben, Debora Berti, Tommy Nylander, Joakim Stenhammar

# DOI

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# **P.160** In situ studies of ancient organic heritage materials and structure in the conservation contexts and environmental-associated preservation

#### Jianlan Wang

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## Abstract

Ancient heritage materials and tangible historic objects typically preserved under extreme and variable environmental conditions, many of them, of organic components, are highly reactive and easily deteriorated in the longer term. Silk textiles, for example, fragile, high selective to ambient humidity and high temperature, lights etc. The relationship between core biomaterial in silk fabric, fibroin, surface structure and biocomposition of materials during degradation and their chemical properties needs to be emphasised in order to understand the mechanisms of ageing and to enable the design of new and better materials for the aim of conservation and restoration. Although studies of the structure, composition, and phase transformation of biomaterial, are challenging, progress has been made in recent years in the development of new techniques across many fields. Through which, new chemistry and new structures of biomaterials with exploration of various surface modification strategy to cope with conservation issues of original materials in complex conditions have been uncovered.

### Last published paper details

Abstract The silk residues in the soil formed the unique niche, termed "silksphere." Here, we proposed a hypothesis that silksphere microbiota have great potential as a biomarker for unraveling the degradation of the ancient silk textiles with great archaeological and conservation values. To test our hypothesis, in this study, we monitored the dynamics of microbial community composition during silk degradation via both indoor soil microcosmos model and outdoor environment with amplicon sequencing against 16S and ITS gene. Microbial community divergence was evaluated with Welch two sample t-test, PCoA, negative binomial generalized log-linear model and clustering, etc. Community assembly mechanisms differences between silksphere and bulk soil microbiota were compared with dissimilarity-overlap curve (DOC) model, Neutral model and Null model. A well-established machine learning algorithm, random forest, was also applied to the screening of potential biomarkers of silk degradation. The results illustrated the ecological and microbial variability during the microbial degradation of silk. Vast majority of microbes populating the silksphere microbiota strongly diverged from those in bulk soil. Certain microbial flora can serve as an indicator of silk degradation, which would lead to a novel perspective to perform identification of archaeological silk residues in the field. To sum up, this study provides a new perspective to perform the identification of archaeological silk residue through the dynamics of microbial communities.

#### Full title of article

Dynamics of microbial community composition during degradation of silks in burial environment

#### Journal

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Abstract The silk residues in the soil formed the unique niche, termed "silksphere." Here, we proposed a hypothesis that silksphere microbiota have great potential as a biomarker for unraveling the degradation of the ancient silk textiles with great archaeological and conservation values.

## All authors

B Wang, C Zhu, Y Hu, B Zhang, J Wang\*

# P.161 Structured emulsion templates: Enabling triple functional porosity in filamentous aerogels

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# Abstract

Interfacial jamming and assembly, facilitated by nanoparticle surfactant (NPS) complexation, demonstrate a remarkable efficacy in stabilizing multiphase systems, evident in structured liquid streams and Pickering emulsions. However, using structured liquid templates to tune multiple porosity levels of ultra-flyweight aerogels has barely been discussed. Herein, we introduced a system spontaneously stabilizing nonpolar droplets within emulsion threads, forming structured worm-like emulsion templates. Specifically, a graphene oxide (GO) emulsion was jetted to hexane as a nonpolar phase in the presence of an active ligand in both the emulsion phase and jetting medium. Thanks to a dual jamming strategy, ultra-flyweight worm-like aerogels are endowed with precisely tailored triple porosity levels. Type I porosities originated from the spaces between filaments, while type II and type III porosities emerged from the evaporation of locked hexane droplets and sublimation of water molecules in the GO emulsion, respectively. The developed aerogels exhibited ultra-low density (1.67-2.3 mg.cm<sup>-3</sup>) coupled with high compressibility (80%), and excellent shape recovery. The intentional creation of multiple porosity levels, along with robust pore structures, conferred these materials with exceptional oil and solvent absorption capacities (e.g., 615 g/g for chloroform), setting new records compared to existing literature. Moreover, the developed aerogels demonstrated an absorption-dominated electromagnetic interference (EMI) shielding mechanism, boasting an exceptional specific EMI shielding (SSE/t) of 67,178 dB cm<sup>2</sup>q<sup>-1</sup>.

# Keywords

emulsion-templating dual interfacial jamming Hierarchical aerogels ultra-flyweight materials

## Last published paper details

Rostami, Sara, Ahmadreza Ghaffarkhah, AliAkbar Isari, Seyyed Alireza Hashemi, and Mohammad Arjmand. "2D nanomaterial aerogels integrated with phase change materials: a comprehensive review." Materials Advances (2023).

#### Full title of article

2D nanomaterial aerogels integrated with phase change materials: a comprehensive review

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# All authors

Sara Rostami , Ahmadreza Ghaffarkhah, Ali Akbar Isari , Seyyed Alireza Hashemi and Mohammad Arjmand

# DOI

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# **P.162** Lipid nanocarriers as potential intranasal delivery vehicles for combination antiretroviral therapeutics to treat HIV

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# Abstract

**Introduction:** Lipid nanocarriers (LN) excel in the delivery of drugs by guarding them against degradation and enhancing their passage through biological barriers, making them favorable candidates for intranasal delivery of antiretroviral therapy (ART) to treat HIV. Yet, their lipophilic interaction with the nasal mucus can hinder penetration. This study aimed to combine two ARTs into an LN (cART-LN) to assess its size, charge, polydispersity, and encapsulation efficiency, in addition to its nasal mucus permeability. The aim was to have an average nanoparticle size of less than 100 nm to bypass the mucus pores, a high encapsulation efficiency of over 80% to minimize spray volume, and a neutral surface charge to minimize interaction with the negatively charged nasal mucus.

<u>Methods</u>: cART-LNs were prepared at 90 °C. Drugs were dissolved in the melted lipid phase. The aqueous phase with a stabilizing surfactant was then added under homogenization, followed by probe sonication. Liquid chromatography measured encapsulation efficiency (EE). Malvern Zetasizer assessed size, polydispersity index (PDI), and surface charge. For nasal mucus permeability and diffusivity studies, a fluorescent model drug replaced the cART. The fluorescent-loaded lipid nanoparticle (F-LN) permeability through the artificial nasal mucus was measured for 3 hours using a Transwell system.

<u>**Results:**</u> All cART-LN and F-LN formulations showed high encapsulation efficiency (>90%), small size (50-65 nm), low PDI (<0.250), and neutral charge (0 to -5 mV). The apparent permeability coefficient ( $P_{app}$ ) through the mucus was 0.55 µm/min, which is considered relatively low permeability.

<u>Conclusion</u>: Lipid-based nanocarriers may offer improved intranasal cART delivery due to their high encapsulation efficiency, small size, monodispersity, and neutral charge. More studies should be done to further enhance the cART-LN's mucus permeability.

# Keywords

HIV Lipid Nanoparticles Combined Antiretroviral Therapy Nasal

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# P.163 Enzymatic modification of yeast mannoproteins for enhancement of emulsification and interfacial properties

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# Abstract

The enzymatic modification of proteins has significant impacts on a protein's capability to create stable emulsions and interact at interfaces. Yeast mannoproteins account for 40% of the yeast cell wall by-products, exhibit high emulsifying properties, and potential for enhancing the bioavailability of encapsulates. In this work, yeast mannoproteins with welldefined structure were isolated from yeast cell wall according to our previous work (Li & Karboune, 2018, 2019) and have been oxidatively crosslinked by laccase from Trametes versicolor to modulate their emulsification and interfacial properties.

Yeast mannoproteins were combined with laccase to achieve varying extents of crosslinking based on reaction time course with ferulic acid as an enhancing phenolic mediator. Emulsification properties of native and modified proteins were evaluated turbidimetrically, interfacial properties were evaluated by the maximum bubble pressure method and the drop volume method

The reaction time courses resulted in enhanced crosslinking based on the enzyme units applied, the reaction length, and the addition of ferulic acid. The extent of crosslinking was reflected in increased molecular weight of protein components at 18h, and a shift favoring the protein fragment in high molecular weight mannan to protein ratio. Mannoprotein modified with ferulic acid had improved emulsion activity index at all pH levels. The interfacial properties were altered significantly. with ferulic acid modified samples showing slower adsorption to the interface and higher equilibrium surface tension. whereas non-ferulic acid modified samples showed lower equilibrium surface tension than native proteins.

Yeast mannoproteins were successfully crosslinked using laccase from T. versicolor with the addition of a phenolic mediator and extent of crosslinking can be controlled by varying the reaction conditions. The modified proteins show promising improvements in emulsification potential and interfacial activity. Understanding the relationship between the extent of crosslinking and the functional properties will provide the capability to generate enhanced protein-containing biopolymer matrices.

# Keywords

Mannoprotein Enzyme

## Emulsifier

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## Full title of article

Emulsion, hydrogel and emulgel systems and novel applications in cannabinoid delivery: A review.

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# All authors

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# **P.164** Self-aggregation, flow behavior and antioxidant activity of microbial biosurfactants: Multifunctionality as the key of eco-sustainable product design

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# Abstract

Microbial biosurfactants are an attractive class of molecules with the potential to replace oil-derived surfactants for the formulation of ecofriendly and biocompatible products. All of them present composite molecular structures, characterized by different functional groups and ionizable moieties and a high conformational flexibility. For this reason, biosurfactants are able to form different aggregates with different morphologies, regulated by a complex interplay between various intermolecular interactions, including H-bonds and steric constraints, besides electrostatic and hydrophobic interactions. In particular, rhamnolipids (Rha) are a type of glycolipid biosurfactants with one or two L-rhamnose units as the headgroup and one or two  $\beta$ -hydroxy-fatty acids as the hydrophobic region. While the micellization of Rha in dilute solutions is well-known, their self-aggregation in concentrated mixtures remains largely unexplored. In this contribution, the emergence of lyotropic liquid crystalline (LLC) phases is analysed both in static conditions and under flow. The experimental investigation (combining POM, SAXS, dNMR, and rheology) is paralleled by a theoretical analysis, with the aim of rationalize the system behavior at a molecular level. Interestingly, electron paramagnetic resonance (EPR) spectroscopy demonstrates the ability of these concentrated mesostructures to stabilize alkoxy radicals. Thus, Rha appear as promising multifunctional components of eco-sustainable formulations, in which not only they can play the typical role of surfactants (i.e., as foaming agents or emulsifiers), but they can also stabilize radical species, thus participating in redox processes, boosting the activity of anti- or pro-oxidant agents.

1. Curr. Opin. Colloid Interface Sci. 2024, in press. https://doi.org/10.1016/j.cocis.2024.101792

2. Colloids Surf. A 2023, 674, 131931.

3. J. Mol. Liq., 2022, 367, 120547.

Biosurfactant Antioxidant Lyotropic Liquid Crystals Rheology

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Ordered hierarchical superlattice amplifies coated-CeO2 nanoparticles luminescence

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# All authors

N. Gallucci, M.-S. Appavou, N. Cowieson, G. D'Errico, R. Di Girolamo, S. Lettieri, F. Sica, G. Vitiello, L. Paduano

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# P.165 Oil binding capacity in low saturated fat matrices using magnetic resonance imaging

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# Abstract

Oil binding capacity (OBC) the ability of fat crystal networks to retain or entrap liquid oils is driven by physicochemical characteristics of the crystalline system formed during processing and post processing. OBC significantly affects the matrix texture and sensory acceptability. A very low OBC can lead to phase separation, and in higher OBC the slow oil movement out of the crystalline network can induce oil migration (OM). OM is directly influenced by the type and concentration of Triacylglycerols, storage conditions, and the crystalline network's solid fat content, polymorphic behavior, micro/nano structure, porosity, and tortuosity. The negative impacts of OM and OBC on food quality is more pronounced in fatty foods made of low saturated fats, and this study aims to model the mechanism of OM in these systems. Using two dilutions of semi-solid Interesterified palm-based fats (IPF) with soybean oil (0%, 50%,) various crystalline networks with a wide range of fatty acid compositions and structural properties were developed. IFP dilutions were crystallized under fast (6.4 °C/min) and slow (0.1 °C/min) cooling rates, as well as with and without the application of high-intensity ultrasound (20 kHz, HIU). Samples microstructure, solid fat content, rheological parameters (G', G'', and  $\delta$ ), melting behavior, and hardness were quantified after 90 min and 48 hours storage at 22 °C and 5 °C. Crystallized samples were placed in contact with 2

layers of tempered cocoa butter and OM between the networks (at the layers interface) was monitored and measured for three months via Magnetic Resonance Imaging (MRI). Sample's experimental oil uptake ratios were used to identify the relationships between the networks' physical and chemical properties and OM, and whether they follow a diffusion-controlled or a relaxationcontrolled mechanism. The research outcome helps the processing design and formulation of healthier food products with acceptable sensory attributes.

### Keywords

MRI NMR Lipid's Crystallization Ultrasouns

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## Full title of article

Unveiling the physical properties predictive of oil binding capacity in an interesterified palm-based fat

#### Journal

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Data From: Unveiling the Physical Properties Predictive of Oil Binding Capacity in an Interesterified Palm-Based Fat Creators Melissa Marsh, Utah State University Brennan Bean, Utah State University Farnaz Maleky, The Ohio State University Silvana Martini, Utah State University

#### All authors

Melissa Marsh, Brennan Bean, Farnaz Maleky, Silvana Martini,

# P.166 Technology of obtaining a superhydrophobic clays from east Kazakhstan's bentonite

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# Abstract

Organoclays obtained by modification of clay minerals have a wide range of applications; they are used as organophilic fillers of paints, regulators or structuring agents of rheological properties of various industrial dispersions.

In this regard, one of the urgent problems is the production of organophilic clays based on domestic Tagan bentonite clays by modifying clay minerals with cationic surfactants containing an amino group. In addition, the possibility of developing ways to obtain modified layered silicate composites based on cationic surfactants will be expanded. There are composites - a material with known strength, thixotropic, deformation properties, which is the basis of drilling fluids, various paints, moisture-resistant coatings, oil sorbents and etc.

The purpose of the work is to develop the possibility of obtaining organoclays from the clays of the Tagan deposit (East Kazakhstan), to develop its technology. Tagan deposit's montmorillonite was used, converted to sodium form to obtain organoclay samples. Tagan deposit's montmorillonite is famous type amount whole clay minerals of Post-Soviet countries due to unique high adsorption properties. At the same time, the purpose of the selected cationic surfactant is to modify the surface of clay particles with a hydrophobic layer as a result of the process of ion exchange with inorganic inter-layer cations of montmorillonite due to the presence of amine groups in the molecular structure. In this scientific work, types of organoclay were obtained with the participation of octadecylamine (ODA).

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#### Keywords

montmorillonite organophylization nanoclays superhydrophobic clays

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# P.167 Study of electrochemical properties of gold nanoparticles and their application in sensors

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Renáta Oriňaková<sup>1</sup>, Ivana Šišoláková<sup>2</sup>, Jana Shepa<sup>2</sup>
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# Abstract

Sensors play a crucial role in diseases diagnostics. They display various advantages such as high sensitivity and specificity, low detection limit, real-time monitoring capability, portability. Especially electrochemical sensors can be used for detection of various biomarkers, such as cancer, cardiovascular diseases, neurological disorders, etc. Gold is frequently used electrode material, that has been widely used due to its chemical stability and favourable electrocatalytic properties. Gold nanoparticles exhibit distinguished electrochemical and photophysical properties, that are closely related to their size. Here screen-printed carbon electrodes (SPCEs) were chosen as the most suitable electrode material for studying the electrochemical properties of Au nanoparticles with different size (8, 20, 40, 60, 80, and 100 nm). It was found that the number and size of particles had great impact on the electrocatalytic activity. The SPCEs modified by gold nanoparticles will be used for the detection of various biomolecules. Among them, dopamine (DA), uric acid (UA) and ascorbic acid (AA) contribute to the healthy functioning of the human body and also act as biomarkers in both independently and coexisting form. According to the preliminary electrochemical measurements SPCEs modified by Au nanoparticles can detect AA in the simulated body fluid. Based on interference and reproducibility study, these electrodes are a promising candidate for use in bioanalyte detection.



Fig.1. Cyclic voltammograms of ferro/ferricyanide depending on size of gold nanoparticles

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# Keywords

electrochemical sensors gold nanoparticles screen printed carbon electrode ascorbic acid

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## Full title of article

NiCoP fibers as novel catalysts for hydrogen evolution in alkali and acidic environment

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# All authors

Cyril Bera, Magdaléna Strečková, Renáta Oriňaková, Alexandra Gubóová, Tomáš Bystroň, Vladimír Girman, František Kromka, Mária Podobová, Karel Bouzek

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# P.168 Block polyampholytes as smart drug carriers for cancer therapy

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# Abstract

Polyampholytes are polymeric systems consisting of both positively and negatively charged monomer subunits. The choice of polyampholytes as smart carriers is based on the hypothesis that one can design such a system that it will undergo self-organization in aqueous media with formations of micellar nanoparticles with hydrophobic interior able to solubilize hydrophobic drug molecules, which will be negatively charged under physiological pH and will be able to reorganize, change the charge to the positive one and release the drug cargo under slightly acidic environment, characteristic for the tumor tissue.

# Polymers with pH sensitive groups



Serie of block amphiphilic copolymers of acrylic acid (AA) and 2-(dimethylamino)ethyl acrylate (DMAEA) were obtained via RAFT (Reversible Addition Fragmentation Chain Transfer) polymerization and demonstrated to act as very efficient drug carriers with good selectivity toward cancers cells. The effect of pH on the size and surface charge of polymeric micellar nanoparticles was studied by dynamic light scattering (DLS) and zeta potential measurements and compared to theoretically calculated values. Drug (doxorubicin) encapsulation efficiency and drug release profile were studied via

fluorescence spectroscopy under physiological and slightly acidic pH. We also assessed cytotoxicity against normal and tumor cells of similar tissue origin like murine 4T1 breast cancer and murine NMuMG mammary gland cell lines.

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## Keywords

polyampholytes drug carriers RAFT polymerization cancer therapy

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All authors

N/A

# P.170 Enhancing antibacterial properties and accelerating in vitro bone regeneration: Synergistic effects of ZnO-loaded bioactive glass/ethylcellulose coatings via electrophoretic deposition on 316L stainless steel

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# Abstract

Addressing the clinical challenge of bone regeneration necessitates a multifaceted approach, including developing biomaterials with osteogenic and antibacterial properties to mitigate post-surgery infection risks. This study focuses on fabricating composite coatings of zinc oxide nanoparticles loaded with CaO-SiO<sub>2</sub>-P<sub>2</sub>O<sub>5</sub>-Na<sub>2</sub>O-B<sub>2</sub>O<sub>3</sub> bioactive glass/ethylcellulose on AISI 316L stainless steel substrates via electrophoretic deposition. The deposition process is conducted in isopropanol suspension with parameters set at 60 V and 5 minutes for voltage and duration, respectively. ZnO nanoparticle loading concentrations of 1 and 2 g/L are employed. Detailed analyses are performed on the microstructure, phase composition, and surface roughness of the coated samples. The physicochemical evaluation confirms the presence of ZnO integrated with the CaO-SiO<sub>2</sub>-

 $P_2O_5$ -Na<sub>2</sub>O-B<sub>2</sub>O<sub>3</sub> bioactive glass/ethylcellulose on AISI 316L stainless steel substrates via electrophoretic deposition. The deposition process is conducted in isopropanol suspension with parameters set at 60 V and 5 minutes for voltage and duration, respectively. ZnO nanoparticle loading concentrations of 1 and 2 g/L are employed. Detailed analyses are performed on the microstructure, phase composition, and surface roughness of the coated samples. The physicochemical evaluation confirms the presence of ZnO integrated with the CaO-SiO<sub>2</sub>-P<sub>2</sub>O<sub>5</sub>-Na<sub>2</sub>O-B<sub>2</sub>O<sub>3</sub> bioactive glass coatings. Corrosion studies in phosphate buffered saline confirm the superior corrosion resistance properties of the coatings over seven days. Additionally, the coatings exhibit a relatively rough surface texture conducive to cell growth (~2.6 µm). Cytocompatibility studies using human placental mesenchymal stem cells demonstrate enhanced cellular viability, attachment, and proliferation on the coated samples. The results indicate acceptable antibacterial efficacy of the ZnO-loaded coatings against *E.coli* and *S.aureus*. Overall, the evaluation of cell viability and assessment of antibacterial properties showcase promising outcomes for the deposited layers.

# Keywords

Bioactive glass Zinc oxide nanoparticles Biomaterial coatings Electrophoretic deposition

# Last published paper details

Hushnaara Hadem, Bangmaya Satpathy, Arijit Mitra, Siddhartha Das, Karabi Das, Optimizing the quality of bioactive glass-polymer coatings through analysis of the effect of dispersing agents on zeta potential and suspension conductivity, Materials Letters, Volume 354, 2024, 135427, ISSN 0167-577X, https://doi.org/10.1016/j.matlet.2023.135427. (https://www.sciencedirect.com/science/article/pii/S0167577X23016129) Abstract: Bioactive glass-polymer (BG-Pol) composite coatings have garnered attention in biomedical applications due to their potential to improve implant performance. This research examines the effects of aluminium nitrate nonahydrate, citric acid, and triethylamine as dispersing agents on the zeta potential and suspension conductivity of BG-Pol suspensions in a 100 % isopropanol suspension. It examines the impact on solutions' electrostatic and conductive behaviour during electrophoretic deposition to enhance coating deposition. The suspensions having a zeta potential above the stability regime (e.g., above 40 mV for polyethylene glycol suspensions) can give a homogeneous coating without dispersants, but below the stability regime, dispersants enable a more uniform coating. The effective deposition was facilitated by a higher suspension conductivity, which exceeded 0.003 mS/cm. Keywords: Bioactive glass; Nanoparticles; Zeta potential; Polymers

# Full title of article

Optimizing the quality of bioactive glass-polymer coatings through analysis of the effect of dispersing agents on zeta potential and suspension conductivity

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Materials Letters

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All authors

Hushnaara Hadem, Bangmaya Satpathy, Arijit Mitra, Siddhartha Das, Karabi Das

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# P.171 Single and poly-crystalline (K,Na)NbO3 heterostructured particles for synergistic photopiezocatalytic Activities

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# Abstract

Piezoelectric materials have been attracting ever-increasing attention in areas like electronics, energy storage, and catalysis due to their non-linear upgrade in performance. In this study, we designed a heterostructure piezo-photocatalyst composed of Ba, Li doped-(K,Na)NbO<sub>3</sub> (KNN) single-crystal microcuboids and CuO nanodots. KNN was selected because of its high piezoelectric coefficient ( $d_{33}$ ), good chemical stability, and environmental friendliness. As a cocatalyst, CuO was considered owing to its advantages such as narrow bandgap, low cost, and nontoxicity. The n-type semiconducting Pb-free KNN single-crystal ferroelectric microcuboids (~30 µm) were synthesized by molten-salt reaction. Then, p-type semiconducting CuO nanodots (less than 5 nm) were uniformly decorated onto KNN microcuboids via deposition of Cu(OH)<sub>2</sub>, followed by conversion to CuO through calcination. From our heterostructure, it is expected that excellent piezoelectric properties could be obtained from KNN single-crystal microcuboids and a high surface area for catalytic reactions is guaranteed by CuO nanodots that are evenly deposited on the surface of KNN without aggregation. The novel KNN/CuO micro/nano heterostructures exhibited increased current density, and enhanced removal organic dye (RhB) efficiencies under the ultrasonic vibration when compared with bare KNN singlecrystal catalysts. Specifically, the reaction rate constant (k) for the photo-piezocatalytic RhB dye degradation of the KNN/CuO micro/nano heterostructure exhibited ~ 0.093 min<sup>-1</sup>, which is higher when compared with other KNN-based piezo, photo, and photo-piezocatalysts. Additionally, the coupled photo-piezocatalyst for KNN/CuO realized an enhanced RhB dye degradation efficiency of 1.6 times and 48.6 times higher when compared with individual piezocatalytic and photocatalytic dye degradation capabilities, respectively. Our approach could provide insights into the design of heterostructure photo-piezocatalysts containing single-crystal ferroelectrics, which requires the enhancement of the photo-piezocatalytic activities.

# Keywords

piezocatalyst niobium oxide photocatalyst photo-piezo catalyst

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Single-Crystal Ferroelectric-Based (K,Na)NbO3 Microcuboid/CuO Nanodot Heterostructures with Enhanced Photo– Piezocatalytic Activity

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E. Im, S. Park, G.-T. Hwang, D. C. Hyun, Y. Min, G. D. Moon

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# P.172 Development of interfaces having dual characteristics and combing solution for combing DNA molecules equivalent to genomic DNA present in single cell

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Suresh Gyanvihar University, Jagatpura, Jaipur, Rajasthan, India. Central University of Punjab, India

# Abstract

We developed different interfaces by using two surface coatings i) Preliminary Coating Surface having positive charge and ii) Secondary hydrophobic coating thus imparting dual characteristics on the glass slide i.e. hydrophobicity alongwith positive charge having affinity for negatively charged molecules such as DNA. Amino group of APTES and APTMS led to positive charge on the preliminary coating surface and the hydrophobic group of secondary coating surface led to high hydrophobicity. Thus, both the characteristics were developed on a single interface. We developed eleven interfaces by two different coatings of which highest deposition efficiency i.e. 42% was observed on PMMA coated over APTES. Thus a surface was developed which had high affinity for combing of single DNA molecules with enhanced retention after post wash conditions. We further developed combing strategies by optimizing the combing solutions to increase fluorescent intensity of the DNA molecules and reduce background fluorescent intensity. We optimized 24 combing solutions, Glycerol: dye molecule ratio was optimized for optimal fluorescence intensity of the combed DNA molecules. Glycerol was observed to increase fluorescent intensity, surfactants besides pH were used for converting single DNA molecules to fibrous state. Combing solutions were optimized for increasing deposition efficiency. DNA equivalent to genomic DNA present in one single human cell was combed over the interface. DNA ssb protein interactions over the combed DNA fibers were, restriction digestion was performed for optical mapping and denaturation of DNA molecules was performed over the surfaces for Fiber FISH. DNA cisplatin adduct formation on the combed DNA fibers were studied. We tried to resolve all the problems associated with DNA combing to make it simple, reproducible and easy to use, and make it applicable for studying replication dynamics, DNA damage response, loop extrusions, stem cell research, DNA replication at early embryonic stage and measuring telomere length.

# Keywords

DNA combing Hydrophobic Surface Deposition Efficiency Replication Dynamics

## Last published paper details

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# Full title of article

Combing of picogram level DNA equivalent to genomic DNA present in single human cell by self propelled droplet motion over a stable gradient surface

#### Journal

Journal of Colloid and Interface Science

#### Year

2024

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## First page

451

# All authors

Hemendra Yadav, Prashant S. Algaonkar, Sudip Chakraborty, Wusirika Ramakrishna

# DOI

https://doi.org/10.1016/j.jcis.2023.11.025

# P.173 Interfacial and bulk properties of similarly charged surfactant-particle binary mixtures

Manaswini , Gowtham V, Sumesh Thampi, <u>Basavaraj MG</u> Polymer Engineering and Colloid Science Lab. Department of Chemical Engineering, IIT Madras, Chennai, India

# Abstract

The addition of surfactants to colloidal dispersions is a simple and effective strategy to tailor the structure and flow properties of multi-component soft-material systems. The amphiphilic surfactant molecules are typically added to colloidal dispersions to engineer their stability and also during the production of emulsions/foams. In this study, we consider association between similarly and oppositely charged surfactant-particle binary mixture in dilute conditions. We evaluate the interfacial and bulk properties of various combinations of particle-surfactant systems to provide comprehensive analysis of particle-surfactant association in such systems. In particular, the nature of complexation in these systems is presented from the measurement of size and surface charge of complexes, surface tension, solution conductivity, critical micellar concentration and by the calculation of surface charge and surface excess concentration.

Self-assembly Particle-surfactant complex Surface Tension Critical Micellar Concentration

## Last published paper details

Reddy, M., Basavaraj, M. G., & Thampi, S. P. (2024). Dynamics of spreading of an asymmetrically placed droplet near a fluid-fluid interface. Soft Matter. 20 (13), 2986-2997

# Full title of article

Dynamics of spreading of an asymmetrically placed droplet near a fluid-fluid interface

#### Journal

Soft Matter

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2024

## Volume

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2986

All authors

Reddy, M., Basavaraj, M. G., & Thampi, S. P.

# DOI

10.1039/D3SM00685A

# P.174 Enhancing CO<sub>2</sub> utilisation process using the novel technique of nanobubbles

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# Abstract

Our planet's future seems bleak with the rising carbon dioxide levels in the atmosphere. Carbon dioxide emissions have become a global concern as it is a primary driver of global warming. While on one hand it has become inevitable to transition to cleaner fuels, however managing the current levels of carbon dioxide is equally important. This is where CO2 utilisation comes into picture. CO<sub>2</sub> utilisation promotes circular carbon economy by converting the waste into value added products, thereby reducing our dependency on the fossil fuels. Various methods have been studied for converting CO2 into valuable products with varying energy demand, yield, cost and selectivity. Out of all the available processes, electrochemical reduction tops the list. Electrochemical reduction of carbon dioxide is the cleanest method to get the desired products using electricity. However, this process is lacking in some aspects such as efficiency and selectivity. Moreover, low CO<sub>2</sub> solubility also hinders this process. The efficiency of the process depends on many factors like, electrode structure, electrolyte concentration, over potential values. This work digs deep into the possibility of using carbon dioxide nanobubbles as the gas source. By incorporating nanobubbles, the solubility has been found to increase by 1.6 times (Fig.2). Carbon dioxide nanobubbles are negatively charged and due to large surface area, heat and mass transfer rates are quite high. This study gives a thorough understanding behind the behaviour of nanobubbles and also investigates the electrochemical reduction process by playing with various parameters like temperature, electrolyte concentration and electrode structure. Also, a comparison has also been made in terms of energy demand and over potential values required for the process. This work concludes on a note that a novel approach has been identified for converting the waste into some useful products by making use of the nanobubble technology.

Nanobubble technology CO2 utilisation electrochemical reduction global warming

## Last published paper details

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## Full title of article

Direct numerical simulation of a single contaminated droplet microextraction in a yield-stress fluid

#### Journal

International Journal of Heat and Mass Transfer

Year

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#### Volume

226

# First page

Direct numerical simulation of a single contaminated droplet microextraction in a yield-stress fluid Shivi Garg, Aakriti Sharma, Jahnavi Mahajan and Neelkanth Nirmalkar

# All authors

Shivi Garg, Aakriti Sharma, Jahnavi Mahajan and Neelkanth Nirmalkar

# P.175 Glycation improved the oxidative stability of myofibrillar protein emulsion: Effect of pH

<u>Jiale Chai</u>, Xinglian Xu, Xue Zhao Nanjing Agricultural University, China

# Abstract

Oxidative stability plays a crucial role in food emulsions that consist of lipids and proteins. Emulsified lipids, particularly polyunsaturated fatty acids (PUFAs) are evidently susceptible to oxidation by free radicals, which lead to a reduction in food quality and nutritional profile of the food products. The glycated myofibrillar protein (MP) with higher solubility and surface hydrophilicity is an available choice for preparation of oil/water emulsions. Especially, the obtained glycation

products provide ability to chelate metals and scavenge free radicals, which regard as potent antioxidants to inhibit oxidation reaction in emulsion. Previously, the continuous cyclic wet heating glycation was carried out to successfully prepare the MP-glucose conjugates, achieving excellent emulsion stability influenced by pH. Furtherly, this study is to investigate the role of glycation on antioxidant ability of glycated MP in soil bean oil-in-water emulsion. The results confirmed that glycation effectively increased the interfacial protein adsorption and emulsification activity of MP.Specially, glycated MP exhibits excellent antioxidant activity at a wide range of pH. Meanwhile, pH significantly affects the oxidative stability of glycated MP emulsions: i) protein oxidation: carbonyl group content is the lowest under neutral condition, while total sulfhydryl content is lowest under alkaline condition; ii) lipid oxidation: the degree of lipid oxidation decreased significantly with the increase of pH. Overall, glycation significantly improves the oxidative stability of MP emulsions in the range of pH 3 to 11, which reveal the internal mechanism of glycation to improve emulsion stability.

# Keywords

Myofibrillar protein glycation oxidative stability pH

# Last published paper details

Chai J., Zhao X., Xu Y., et al. An unfolding/aggregation kinetic instructed rational design towards improving graft degree of glycation for myofibrillar protein [J]. Food Chemistry, 2024, 446:138876.

# Full title of article

An unfolding/aggregation kinetic instructed rational design towards improving graft degree of glycation for myofibrillar protein

# Journal

Food chemistry

Year

2024

# Volume

446

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138876

# All authors

Jiale Chai, Xue Zhao, Yujuan Xu, Xinglian Xu

# **P.169** Synthesis of a pH responsive polymeric ligand for selective adsorption of Uranium (VI) from alkaline leach liquor

<u>ABHIJIT DAS</u>, Sirshendu De Indian Institute of Technology Kharagpur, India

# Abstract

The modern energy revolution has come, with environmentally friendly and reliable nuclear energy emerging as one of the finest fossil fuel substitutes without depleting greenhouse gasses like,  $CO_2$ , etc. In this work, alkaline leaching is used for the selective extraction of carbonate ore. A hyper-branched cross-linked polymeric ligand was synthesized using the free radical co-polymerization of acrylamide and N, N-methylene bisacrylamide. In addition, potassium persulfate (as initiator) and dodecanethiol (as brancher) were used to transfer the radicals for faster chain formation and smooth branching of the long chain polymer. The Langmuir maximum U adsorption capacity of polymeric adsorbent was 1007 mg/g at 303 K and 98.4 % of U was removed from alkaline leach liquor. U was adsorbed at pH 8.3 in presence of various interfering co-ions and desorbed at pH 11 in the form of sodium diuranate (Na<sub>2</sub>U<sub>2</sub>O<sub>7</sub>) precipitate. The adsorption was monolayer, exothermic and spontaneous in

nature. The C-N, CO-NH<sub>2</sub> and OH groups of adsorbent interacted with uranyl ions  $(UO_2^{2^+})$  initiating the coordinative and electrostatic interactions leading to U adsorption. Continuous fixed bed column runs were performed using the actual leach liquor and a fundamental model was used to quantify the performance of the columns. The transport parameters were estimated from the model and scaling up calculations were performed using these parameters. Five adsorption-desorption cycles were conducted to determine the reusability and structural stability of the synthesized polymeric adsorbent. Also, the structural stability was confirmed of the developed polymeric ligand by TGA (thermal stability) and NMR (cross-linked stability) analysis.

# Keywords

Adsorption Co-ordinative interaction Criss-linked polyemer Thermal stability

# Last published paper details

Das, A., Roy, D., Erukula, K., De, S., 2024. Synthesis of pH responsive malononitrile functionalized metal organic framework MIL-100(Fe) for efficient adsorption of uranium U(VI) from real-life alkaline leach liquor. Chemosphere 348, 140780. https://doi.org/10.1016/j.chemosphere.2023.140780

# Full title of article

Synthesis of pH responsive malononitrile functionalized metal organic framework MIL-100(Fe) for efficient adsorption of Uranium U(VI) from real-life alkaline leach liquor

# Journal

Chemosphere

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2024

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348

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Synthesis of pH responsive malononitrile functionalized metal organic framework MIL-100(Fe) for efficient adsorption of Uranium U(VI) from real-life alkaline leach liquor

## All authors

Abhijit Das, Debashis Roy, Karthik Erukula, Sirshendu De

# DOI

10.1016/j.chemosphere.2023.140780

# P.176 Amino acid-based thermo-responsive hydrogel/MOF/CaCl<sub>2</sub> composites for atmospheric water harvesting

<u>Sandeep Kumar Sahoo</u> Indian Institute of Technology Delhi, India

## Abstract



畅 Water moisture 🛛 🛶 Swollen polymer 🛛 🥧 Dried polymer 🝵 Al<sub>m</sub> MOF

The innovative approach based on sorption-based water harvesting involves extracting moisture from the atmosphere, mitigating water scarcity, and establishing a sustainable means of obtaining clean water. The amino acid-based hydrogels are known for their ability to absorb and retain water effectively due to their hydrophilic nature, responsiveness, and biocompatibility. Incorporating Metal-Organic Frameworks (MOFs) and CaCl<sub>2</sub> into hydrogel matrices is a prevalent approach, resulting in a range of hydrogel/MOF/CaCl<sub>2</sub> composites exhibiting enhanced sorption characteristics. The combination of MOF's rapid hydration and superior breathability with hydrogel's hydrophilic properties and large water retention capacity make these composites a promising alternative for extracting water from the atmosphere. The present study concentrates on the latest advancements in the techniques employed for the synthesis of MOFs, hydrogels, and hydrogel-MOF/CaCl<sub>2</sub> composites, and a comprehensive analysis of the advantages and disadvantages of each approach

with the capacity reaching 1.79 gg<sup>-1</sup> at approximately 90% RH and 30°C within 24 hours and reaching 3.16 gg<sup>-1</sup> of maximum absorption capability. The composite also exhibits outstanding durability, low desorption temperature (approximately 35±5°C, the lowest), and high water-releasing rate, releasing 98% of the sorbed water under 40°C and 60% RH for only 2 hours. This hydrogel-MOF composite has the potential to significantly impact various industries, including water treatment, desalination, and moisture harvesting.

# Keywords

Thermo-responsive hydrogel Atmospheric water harvesting Sorption-based water harvesting Hydrogel Composite

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First page
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# P.177 High-throughput 3D cardiac spheroid biochip via particle array method

Jae-Hyeok Lee, Seri Choi, Eun-Mi Kim, Ki-Suk Kim Korea Institute of Toxicology, Republic of Korea

# Abstract

The importance of evaluating the safety and efficacy of medicines using cardiomyocytes, brain cells, and hepatocytes derived from human stem cells is drawing attention. Since the two-dimensional (2D) single-layer cell culture substrate is placed in a very different environment from the actual in-vivo system, cells tend to rapidly lose their intrinsic characteristics, and it becomes difficult to control stem cell differentiation. Spheroids (cell aggregates) produced via threedimensional (3D) cell culture methods have attracted an increasing amount of interest in the field of drug screening due to the significant advantages associated with more accurate simulation of their in-vivo behavior compared to two-dimensional culture methods. Conventional techniques for preparing spheroids include hanging drops, concave microwell aggregates, spinner flasks, and gravity cycling. However, all these methods have limitations such as low scalability, low viability, loss of spheroids, and irregular size distribution. To overcome these limitations, in this study, high-throughput 3D cardiomyocyte spheroids were efficiently fabricated using biocompatible RGD peptide-coated silica nanoparticles (700 nm). The RGD functionalized silica nanoparticles were then densely-packed arrayed in a monolayer on a non-fouling polymer,

## Keywords

Biochip
Drug screening
3D spheroid
Diagnosis

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First page

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All authors

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# P.178 Rheological properties of sodium N-acyl sarcosinate solutions

<u>Dilek Gazolu-Rusanova</u>, Marina Stoeva, Slavka Tcholakova Department of Chemical and Pharmaceutical Engineering, Faculty of Chemistry and Pharmacy, Sofia University, Bulgaria

# Abstract

Sarcosinates are amino acid based anionic surfactants with excellent adsorption and foaming properties, low toxicity, high biodegradability, broad biological activity and mildness to the skin. This class of natural surfactants have attracted considerable attention as potential substitutes for sulfate containing surfactants (e.g. SLES) in cosmetic products. In this study the influence of the type and concentration of electrolyte, the addition of co-surfactants, and the length of the hydrocarbon tail on the rheological behavior of solutions of sodium alkyl sarcosinates with a total concentration of 10 wt% was systematically investigated. The obtained results showed that the viscosity of the solutions increases with the increase of electrolyte concentration until the concentration for phase separation is reached,  $C_{\rm TR}$ . The concentration of electrolyte for inducing micelle growth,  $C_1$ , and for precipitation,  $C_{\rm TR}$ , decrease with increasing hydrocarbon chain length and with increasing counterion size. Zwitterionic co-surfactants, cocoamidopropyl betaine (CAPB), sulfobetaine or decylamine oxide do not change the general appearance of the salt curve, but lead to an increase in  $C_{\rm TR}$  and a change in the maximum viscosity that can be reached before precipitation. We hypothesized that mixed micelles are formed with cAPB+sodium lauroyl sarcosinate that are not significantly different from micelles of sarcosinate alone because in both cases carboxyl groups remain on the surface of the micelles. When using amine oxide, separate micelles of sarcosinate, which, however, cannot grow sufficiently due to its reduced concentration in the mixture. It was found that the addition of

# Keywords

sodium N-acyl sarcosinate phase behavior viscosity salt curves

## Last published paper details

Dilek Gazolu-Rusanova, Ivan Lesov, Slavka Tcholakova, Nikolai Denkov, Badreddine Ahtchi, Food grade nanoemulsions preparation by rotor-stator homogenization, Food Hydrocolloids, Volume 102, 2020, 105579, ISSN 0268-005X, https://doi.org/10.1016/j.foodhyd.2019.105579. (https://www.sciencedirect.com/science/article/pii/S0268005X19315565) Abstract: High-pressure homogenizers, typically used for producing nanoemulsions at the industrial scale, are energy and maintenance intensive, and limited to produce only dilute, low viscosity nanoemulsions. We propose an alternative approach to produce dilute to concentrated food-grade nanoemulsions with droplet size ranging between 100 and 500 nm using rotor-stator homogenization. Gum Arabic (GA) or modified starch (MS) was used as both viscosity modifier and emulsion stabilizer. GA and MS have relatively low surface activity compared to the common low-molecular-mass surfactants used typically for nanoemulsion preparation. The main differences between GA and MS are the lower viscosity of the GA solutions, compared to MS solutions, and the faster adsorption of MS, as compared to GA. The obtained results show that stable nanoemulsions are formed by rotor-stator homogenization when the rapidly adsorbing MS is used as emulsifier. Much larger drops are formed during emulsification with GA, which is due to significant drop-drop coalescence in the respective emulsions. The experimental results for the nanoemulsions prepared with MS are well-described by the theoretical expression for emulsification in turbulent viscous regime, after proper account for the effects of temperature and drop-drop interactions in the sheared emulsions. Keywords: Nanoemulsions; Rotor-stator homogenizer; Modified starch; Gum Arabic; Drop size; Drop size prediction

## Full title of article

Food Grade Nanoemulsions Preparation by Rotor-Stator Homogenization

Journal

Food Hydrocolloids

Year

2020

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105579

#### All authors

Dilek Gazolu-Rusanova, Ivan Lesov, Slavka Tcholakova, Nikolai Denkov, Badreddine Ahtchi

# DOI

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# **P.179** Temperature response of sucrose palmitate solutions: Role of ratio between monoesters and diesters

<u>Nevena Pagureva<sup>1</sup></u>, Diana Cholakova<sup>1</sup>, Zlatina Mitrinova<sup>1</sup>, Nikola Burdziev<sup>2</sup>, Slavka Tcholakova<sup>1</sup>

<sup>1</sup>Department of chemical and pharmaceutical engineering, Faculty of chemistry and pharmacy, Sofia university, Bulgaria. <sup>2</sup>Faculty of chemistry and pharmacy, Sofia university, Bulgaria

# Abstract

Aqueous solutions of long-chain water-soluble sucrose ester surfactants exhibit non-trivial response to temperature variations, revealing a peak in viscosity around 40-50°C. While previous investigations have explored the structures within sucrose stearate systems at various constant temperatures, a comprehensive understanding of the entire temperature dependence and the underlying molecular factors, contributing to this phenomenon is currently missing.

We examine the temperature dependent properties and supramolecular structures formed in aqueous solutions of commercial sucrose palmitate surfactant using cryo-TEM and optical microscopy, rheological measurements, NMR, SAXS/WAXS, and DSC.

The experimental results reveal the intricate role of the mono- and di-esters ratio in solution on its overall properties. Solutions, primarily containing sucrose monoesters, exhibit behavior typical for non-ionic surfactants, with minimal changes with temperature. In contrast, the coexistence of mono- and di-esters results in the formation of discrete monodisperse diester particles coexisting with a network of partially fused diester particles at low temperature. As the temperature approaches the diesters' melting point, wormlike mixed micelles form, causing a viscosity peak, yet some diester particles persist in the solution. Further temperature increase leads to fluidization of surfactant tails and formation of branched micelles, whereas the excess diester molecules phase separates into distinct droplets.

## Keywords

Sucrose monoester/diester phase behavior at different temperatures rheology biodegradable surfactant

## Last published paper details

Slavka Tcholakova, Fatmegul Mustan, Nevena Pagureva, Konstantin Golemanov, Nikolai D. Denkov, Edward G. Pelan, Simeon D. Stoyanov, "Role of surface properties for the kinetics of bubble Ostwald ripening in saponin-stabilized foams", Colloids and Surfaces A: Physicochemical and Engineering Aspects, Volume 534, 2017, Pages 16-25, ISSN 0927-7757, https://doi.org/10.1016/j.colsurfa.2017.04.055. Highlights • Main reason for the slow bubble coarsening is high resistance of adsorption layers to gas diffusion. • Deviations from the equilibrium surface tension have noticeable but smaller effect. • Rate of bubble OR correlates with the surface stress, measured at very low deformation rates. • Gas flux across the meniscus region is accounted by new theoretical expression. • Flux across the meniscus region is important for single bubbles and at low bubble volume fraction.

#### Full title of article

Role of surface properties for the kinetics of bubble Ostwald ripening in saponin-stabilized foams

#### Journal

Colloids and Surfaces A: Physicochemical and Engineering Aspects

#### Year

2017

#### Volume

534

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16

#### All authors

Slavka Tcholakova, Fatmegul Mustan, Nevena Pagureva, Konstantin Golemanov, Nikolai D. Denkov, Edward G. Pelan, Simeon D. Stoyanov

#### DOI

https://doi.org/10.1016/j.colsurfa.2017.04.055

# P.180 Decellularized pulmonary extracellular matrix-based hydrogel for 3D culture of small cell lung cancer cells

<u>Chang Seok Ki</u>, Yoobin Han, Mijung Jung, Yujin Kong Seoul National University, Republic of Korea

# Abstract

Small cell lung cancer (SCLC) is one of lethal cancers leading to aggressive invasion and poor prognosis, resulting in an extremely low 5-year survival rate. Unlike common cancers that form solid tumors, SCLC's stages are divided into limited and extensive stages. Unfortunately, both diagnosis and surgical operation are not successful in any stages and the average survival span of SCLC patients is only 9 months from the first diagnosis. Hence, its treatment relies on chemo-and radio-therapies. The related research is being conducted based on old-fashioned cell culture platform (suspension & monolayer), although diverse culture technologies (e.g., spheroid, scaffold, gel, 3D bioprinting) are tried for other cancer cells. In general, dECM of a specific tissue contains essential components for cell attachment and biological cues. Thus, dECM-based materials are widely used as matrices for 3D cell culture. In this work, for 3D culture of SCLC cells, a hydrogel matrix is formed with decellularized porcine pulmonary extracellular matrix (dECM). For photo-crosslinking, the isolated dECM is modified with methacrylate group and hybridized with hyaluronic acid in order to compensates the loss of glycosaminoglycans during the decellularization. The encapsulated SCLC cells in dECM hydrogel well proliferate and exhibit cancer stem cell (CSC)-like phenotype. Interestingly, the CSC phenotype is dependent on the matrix stiffness that is controlled by crosslinking density. In addition, the invasiveness of encapsulated cells can be evaluated quantitatively using the dECM hydrogel. Conclusively, the obtained results indicate the dECM hydrogel is a proper 3D culture platform to assess drug sensitivity and malignancy of SCLC cells.

# Keywords

small cell lung cancer decellularized extracellular matrix hydrogel 3D culture

# Last published paper details

Y. Han, C. S. Ki, Macromolecular Bioscience (2024) 24(3), 2300356

# Full title of article

Effect of matrix stiffness and hepatocyte growth factor on small cell lung cancer cells in decellularized extracellular matrixbased hydrogels

# Journal

Macromolecular Bioscience

Year

2024

# Volume

24

# First page

2300356

# All authors

Y. Han, C. S. Ki

# P.181 Force-extensions relationships for grafted active colloidal filaments and chains

Arvind Gopinath<sup>1</sup>, Prashant Purohit<sup>2</sup>

## Abstract

We study the mechanical properties of stretched elastic chains and filaments comprised of connected active colloids. Changes in chain configurations arise from a combination of thermal Brownian noise and stochastic non-thermal active noise. Analytical force-extension relationships for chains and filaments under experimentally motivated boundary conditions are derived and compared to corresponding expressions for passive elastic chains. We show that for certain limiting cases, the force-extension relationship resembles the classical result for worm like chain (WLC) polymers with activity-dependent elastic moduli and temperature.

## Keywords

Active colloids WLC Temperature Fluctuations

#### Last published paper details

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# Full title of article

Facile determination of the Poisson's ratio and Young's modulus of polyacrylamide gels and polydimethylsiloxane

#### Journal

ACS Applied Polymer Materials

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# **First page**

2405

# All authors

Ariell Marie Smith, Dominique Gabriele Inocencio, Brandon Michael Pardi, Arvind Gopinath, Roberto Carlos Andresen Eguiluz

# DOI

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# P.182 Creation of in-situ spontaneous formation of menthoxypropanediol loaded niosomes for cosmetic application

Xin Yen Chiang, Kah Huong Chong, Norsyariza A.Aziz, Timothy Tze Chun Ting, Ka-Heng Lee, Khan Loon Ng, Mong Sah Toh

Winnox Cosmeceutics Sdn Bhd, Malaysia

# Abstract

Niosomes is characterized as non-ionic surfactant vehicles with advantages to form nano vesicles without need of external energy, unlike liposomes that typically require highpressure homogenization. This distinctive feature has led to a growing significance of niosomes in cosmetic applications due to their commercial viability. Their ease of

development has offered a cost-effective means to encapsulate actives molecule, enhancing their penetration into the skin and facilitating a slow-release mechanism for prolong effect on skin.

In this study, an in-situ spontaneous formation of niosome was successfully created for cosmetic application using a combination of mannosylerythitol lipids, peg-40 hydrogenated castor oil, sodium stearoyl glutamate and glycols. The niosomes were then characterized based on their particle size, surface charge, polydispersity index using dynamic light scattering (DLS). Additionally, their morphology properties were evaluated using wide angle X-ray scattering (WAXS) and Transmission electron microscope (TEM). The results showed that the niosome fell into the categories of small unilamellar vehicles (SUV) with an average size of 43.83nm and a narrow polydispersity of 0.171 nm. The TEM and WAXS analyses confirmed the spherical morphology of the niosome and was consistent with the size measured obtained from DLS.

The technology was applied to encapsulate menthoxypropanediol (MP), an interesting molecule known for its cooling sensation, especially beneficial in hot and humid climatic applications. Upon loading of the target molecule, an increase in the particle size to 91.9 nm was observed. Validation of menthoxypropanediol content was performed using ultraperformance liquid chromatography (UPLC), demonstrating a recovery of active level exceeding 90%. To evaluate the performance of MP loaded niosomes, a skin penetration profile was studied using ex-vivo human skin, revealing a controlled release profile of 2 hours at rate 1.5 ratio slower than control. Stability studies conducted at 45 C over 3 months showed the MP-loaded niosomes remain structurally intact.

# Keywords

Niosomes Menthoxypropanediol Encapsulation Mannosylerythitol

# Last published paper details

P.Y. Lau, K.L. Ng, N.A. Yusof, G. Liu, Y. Alias, S.M. Khor, A sample pre-treatment-free electrochemical immunosensor with negative electro-pulsion for the quantitative detection of acrylamide in coffee, cocoa and prune juice, Analytical Methods. 11 (2019) 4299–4313. https://doi.org/10.1039/c9ay01102a.

# Full title of article

Sample pre-treatment free electrochemical immunosensor with negative electro-pulsion for quantitative detection of acrylamide in coffee, cocoa and prune juice.

# Journal

Analytical methods

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2019

# Volume

11

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## 4299

## All authors

Pei Ying Lau, Khan Loon Ng, Nor Azah Yusof, Guozhen Liu, Yatimah Alias, Sook Mei Khor

# P.183 Deposit control in cosmetic systems for optical fine tunning performances

<u>Guillaume Votte</u> L'Oréal, France

## Abstract

Skincare products are mostly used to improve the appearance and state of the skin based on biological and physical effects. Optical effects are of major importance in these expected benefits for consumers. They are generally conveyed by the addition of

particles/fillers with intrinsic optical properties. Adding these particles in significant

quantities to maximize these optical performances may have a negative impact on the sensorial attributes and application qualities. Today, formulators, and consequently users, have to make a

compromise between optical effect performance (mattity, blurring, coverage...),

and sensorial attributes (product texture, comfort, smoothness, homogeneity, playtime upon application). The understanding of the organization within the deposit is necessary to be able to drive the final properties. In this study, we focus on the relationship between the structure of the deposit and its optical properties, especially the mattity. We developed a methodology to characterize surfaces with standards models and then we applied this methodology to decode complex colloidal systems such as cosmetic formulation.

## Keywords

Cosmetic deposit sciences topography optic

Last published paper details

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Year

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All authors

N/A

P.184 Biodegradable nanocellulose-based coating for transparent food packaging

## Korea Institute of Science and Technology, Republic of Korea

## Abstract

As the demand for single-person household-sized food packages continues to rise, the development of advanced food packaging materials becomes increasingly crucial. This study presents an innovative approach to address this need, focusing on the creation of sustainable and effective food packaging solutions. We introduce a novel method involving dialdehyde-modified cellulose (DAC) blended with polyvinyl alcohol (PVA), applied onto PLA films using the doctor blade coating method. This eco-friendly, scalable process leads to the formation of films with exceptional gas barrier properties.

These films not only offer superior gas barrier performance but also possess key environmentally friendly attributes. They are fully biodegradable, eliminating concerns related to their end-of-life disposal. Furthermore, these films demonstrate optical transparency, allowing consumers to easily identify packaged products. Additionally, their radio frequency identification (RFID) transparency opens up possibilities for improved inventory management and traceability in the food supply chain.

Our research findings suggest that these PLA/*h*-DAC-PVA films hold great promise as eco-friendly food packaging materials. By effectively preserving food quality and extending shelf life, these coatings contribute to environmental responsibility in the food industry. This study presents a significant step toward sustainable food packaging solutions that meet the needs of both consumers and the environment.

## Keywords

nanocellulose thin films barrier films biodegradable

## Last published paper details

ACS Appl. Polym. Mater. 2024, 6(7), 4050-4059.

### Full title of article

Self-healable and degradable polycarprolacton-based polymeric binders for lithium ion batteries

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# All authors

Lim, Taeho; Yoon, Jiyoung; Lee, Chulyong; Baek, Kyung-Youl; Jeon, Ju-Won; Cho, Sangho

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# P.185 Mucoadhesive lecithin-chitosan hybrid nanoparticles confer improved oral bioavailability, enhanced in-vitro efficacy and safety to dasatinib

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# Abstract

**Introduction:** Dasatinib (DAS) has established antiproliferative activity in triple-negative breast cancer. However, its efficacy is significantly subsided by its low oral bioavailability and first-pass metabolism. Chitosan is a cationic mucoadhesive polymer that prolongs the residence time by interacting with the mucin layer. In pursuit of improving the oral delivery of DAS, mucoadhesive lecithin-chitosan hybrid nanoparticles (DAS-L/CS-NPs) were fabricated.

**Methods:** The DAS-L/CS-NPs were prepared by nanoprecipitation and optimized by the Box–Behnken design. These NPs were characterized for mean particle size, zeta potential, entrapment efficiency and morphology. PXRD, FTIR analysis and stability studies were also conducted. *In-vitro* drug release at different pH conditions, ex-vivo drug permeation and ex-vivo mucoadhesion studies were executed. Further, *in-vitro* cell-based assays in MDA-MB-231 cells were conducted to appraise the efficacy of NPs. *In-vivo* pharmacokinetic study and acute toxicity study of DAS-L/CS-NPs were performed.

**Results:** The optimized DAS-L/CS-NPs exhibited mean particle size and zeta potential of 179.7 ± 5.16 nm and 37.67 ± 2.38, respectively. DAS-L/CS-NPs demonstrated sustained release profiles in different release media up to 48 h and 10 times higher apparent permeability coefficient than free DAS. Further, DAS-L/CS-NPs showed a 10.27-times higher concentration of DAS in the rat intestinal mucosal layer than free DAS. Further, DAS-L/CS-NPs revealed a 4.08-fold decrease in IC<sub>50</sub> and significantly higher cellular uptake, increased reactive oxygen species generation, mitochondrial membrane depolarization and apoptosis in MDA-MB-231 cells than free DAS. Moreover, DAS-L/CS-NPs showed a 5.08-fold rise in AUC<sub>(0-t)</sub> than free DAS. Histological examination and plasma marker analysis indicated less toxicity in vital organs.

**Discussion:** DAS-L/CS-NPs showed mucoadhesion owing to the interaction between chitosan and mucin. Thus, DAS-L/CS-NPs exhibited enhanced oral delivery owing to mucoadhesion, increased residence time and absorption. In a nutshell, the developed nanocarrier bestowed augmented oral bioavailability, efficacy and safety to DAS.

# Keywords

Mucoadhesion Hybrid-nanocarrier Dasatinib Chitosan

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#### Full title of article

Dasatinib loaded mucoadhesive lecithin-chitosan hybrid nanoparticles for its augmented oral delivery, in-vitro efficacy and safety

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## All authors

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# P.186 Gallium-based composite PCM for battery thermal management

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## Abstract

This paper presents an experimental investigation of gallium-based composite phase-change materials (CPCMs) for the thermal management of lithium-ion batteries (LIB) under fast charging/discharging conditions. CPCMs were prepared by mixing paraffin (PA), gallium (Ga), and expanded graphite (EG) in different ratios, and their thermal properties were characterized by differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and thermal conductivity measurements. The CPCMs were then applied to a cylindrical battery cell, and the temperature profiles were monitored at various discharge rates. The results indicated that CPCMs with a higher proportion of Ga exhibited lower melting temperatures, higher thermal conductivities (101 times compared with pure PA), and better thermal stability than pure paraffin-based PCM.

# Keywords

Batteries Thermal management Heat transfer Phase change materials

#### Last published paper details

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# Full title of article

Advancements in Battery Thermal Management System for Fast Charging/Discharging Applications

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**Energy Storage Materials** 

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Battery energy storage systems (BESS) are essential for integrating renewable energy sources and enhancing grid stability and reliability.

# All authors

Shahid Ali Khan, Iftikhar Hussain, Amrit Kumar Thakur, Shi Yu, Kwun Ting Lau, Sihong He, Kejian Dong, Jingtan Chen, LI Xiangrong, Muhammad Ahmad, Jiyun Zhao

# DOI

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# P.187 One-step synthesis of carbon dots designed for advanced multiparametric bioimaging probe applications

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# Abstract

Carbon dots (CDs) have recently emerged in biomedical and agricultural domains, mainly for their probe application for developing efficient sensors. However, the existing hightemperature approaches limit the industrial level scaling up to further translate it into different products by mass-scale fabrication of CDs. To address this, we have attempted to lower the synthesis temperature to 120°C and synthesized different CDs using different organic via condensation mechanism. The material was characterized by detailed analyses, such as, FTIR, UV–visible absorption and photoluminescence spectroscopies, XRD, HRTEM, and zeta potential. Further, sensing applications of CDs have been explored in biological models like bacterial strains and the *Lactuca sativa* (lettuce) plant. Bacterial bioimaging experiments revealed CD compatibility with gram-positive and gram-negative strains without bactericidal effects. Furthermore, CDs demonstrated effective conduction and fluorescence within the vascular system of lettuce plants, indicating their potential as *in vivo* probes for plant tissues. The bioimaging of CDs in different biological models indicates the possibility of developing a CD probe for diverse biosensing roles in diseases, metabolism, microbial contamination sensing, and thereof.

# Keywords

Carbon Dots One-Step Synthesis Bioimaging Plant Bioimaging Probes

#### Last published paper details

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# Full title of article

Polyurethane Chemistry for the Agricultural Applications - Recent Advancement and Future Prospects

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## All authors

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## DOI

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# P.188 ISIS-II – a potential future neutron source for the colloid community

#### Sarah Rogers

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## Abstract

Neutron scattering is powerful technique for studying a wide variety colloidal system as it can be used to determine both spatial and temporal information of multicomponent systems at the nanoscale [1, 2]. Instrument Scientists at the ISIS Neutron and Muon Source already work closely with the Colloid Community exploiting both diffraction and spectroscopic techniques such as small-angle scattering (SANS), neutron reflectometry (NR) and quasi-elastic neutron scattering (QENS) to study a broad range of systems across a large size and time regime.

Building on the success of the current source, a new more powerful (MW) facility, ISIS-II, is currently being investigated, with the aim of starting construction from the early 2030s. The UKRI infrastructure fund has supported the initial feasibility studies for ISIS-II and an award of around £5m has enabled initial work on the accelerator and target options, together with development of the overall case for the facility. This source will be complementary to other neutron facilities available to the community and will add both capacity and capability.

Further, more details, feasibility work is required and as part of this, a detailed review of the science opportunities is underway which will further inform the accelerator and target stations options analysis.

Here, potential facility designs will be presented with details of what parameters could be achieved, such as the size regime, the dynamic and time ranges covered, as well as what new instrument techniques could be developed. It is also an opportunity for the colloid community to feed it's future requirements into this project.

- 1. A Practical Guide to Quasi-elastic Neutron Scattering, M T F Telling
- 2. Colloid Science. Principles, methods and applications, T Cosgrove

### Keywords

Neutrons Scattering Multicomponent

## Last published paper details

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#### Full title of article

A Facile Surfactant-assisted Synthesis of Graphene Oxide/Zinc Oxide Catalyst for the Degradation of Methylene Blue Dye

## Journal

Water Air and Soil Pollution

## 2024

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# All authors

M M H Abdul Aziz, A Mohamed, T Ardyani, S A Bakar, M Sagisaka, K Sato, M K Ahmad, R Nuryadi, S E Rogers

# DOI

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# P.189 Predicting surfactant properties with graph machine learning

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# Abstract

Predicting surfactant properties through computer-aided methods can accelerate the search for new sustainable surfactants with reduced experimental efforts. Classical quantitative structure-property relationship (QSPR) models have been successfully developed and applied in predicting surfactant properties such as the critical micelle concentration (CMC), the hydrophile-lipophile balance (HLB) and the surface excess concentration (Гm). Recently, graph-based machine learning (ML), specifically graph neural networks (GNNs), have been successfully applied to predict the CMC of surfactants at a constant temperature. Compared to classical QSPR models, GNNs operate directly on the molecular structure, automatically extracting structural features and correlating them with the CMC in an end-to-end learning framework. However, capturing the temperature effect on CMC or simultaneously predicting multiple surfactant properties to overcome data availability limitations has not yet been investigated.

We present two developed GNN models; a) for predicting multiple surfactant properties at a constant temperature and b) for predicting the CMC of surfactants at varying temperatures. The first GNN model accurately predicts the CMC and surface excess concentration of surfactant molecules at a constant temperature. The results show that simultaneously learning multiple surfactant properties with one GNN, referred to as multi-task learning, substantially improves the model accuracy for properties where data is lacking. We also apply the GNN model to three industrial-grade surfactants and obtain highly accurate predictions, thus demonstrating a potential use-case in industrial applications. The second GNN model performs highly accurate CMC predictions for surfactant molecules at various temperatures. We demonstrate the high predictive ability of the model under different test scenarios, namely surfactants previously seen at different temperatures. The two GNN models, can be used as an initial screening tool in the research for new sustainable surfactants with desired properties.

# Keywords

Surfactants Graph neural network critical micelle concentration temperature-dependency

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Graph neural networks for surfactant multi-property prediction

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# DOI

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# P.190 Nickel/N-doped carbon nanocomposite as electrode material for supercapacitor application

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# Abstract

Covalent organic frameworks (COFs) are gaining high importance in energy storage systems due to their uniform porosity and versatile functionality. The present work deals with the fabrication of triazine-based COF through Schiff base formation. The covalent triazine framework was further doped with nickel using the wet impregnation method. The material was further carbonized at 700 °C to give Ni@ N-doped carbon. The material was characterized for its morphology, crystallinity, structure, and porosity. The pristine COF, N-doped carbonized COF, and Ni@N-doped carbonized COF were used for supercapacitor application. The materials were studied for charge storage applications in three-electrode cell and in symmetrical two-electrode supercapacitor device. An enhanced specific capacitance was observed on doping the Ndoped carbonized COF with Ni.

# Keywords

Triazine based Covalent organic framework Supercapacitor Nickel doping Energy storage system

# Last published paper details

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# Full title of article

Ultrafast adsorption of hexavalent chromium from aqueous effluents using covalent triazine frameworks

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Chemosphere

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2024

# First page

We have synthesized low-cost high performance covalent triazine framework (CTF) through Schiff base reaction of melamine and terephthalaldehyde with different proportions of the reactants. The synthesized adsorbents showed excellent capacity for adsorption of Cr (VI) at acidic pH while almost negligible adsorption at higher pH.

# All authors

Olviya S. Gonsalves, Parag R. Nemade

# DOI

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# P.191 When physical chemistry helps circular economy: Residues from pyrolysis of urban wastes can improve asphalts performance

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# Abstract

Experiment: A circular use of residues (bio-oil and char) from municipal waste pyrolysis is proposed for producing improved asphalts and for their regeneration when aged.

Two char samples, deriving from the pyrolysis of two different wastes (refuse solid waste, RDF, and waste tyre rubber, WTR) were used for the preparation of bitumens samples. Rheological tests have been performed to determine the mechanical properties of neat bitumen and char-modified bitumens. Preliminary results revealed a higher temperature resistance and a reinforcement of the overall chemical structure of the char-modified bitumens (Figure 1).

351


Figure 1: tan d as a function of temperature for the three bitumen samples.

Measurements to evaluate possible anti-aging effects have been also performed. The addition of bio-oil can restore in part the original viscosity of an aged bitumen.

Interpretation: Char carbonaceous particles have good chemical compatibility with the bitumen chemical nature so they can be well accommodated giving increased load capacity and decrease in the formation of cracks. In addition, small particles in a bitumen can act as solid barriers towards the asphaltene diffusion (hindered dynamics) hindering their self-assemble and reducing the overall bitumen aging. Finally, the liquid fraction of pyrolysis residue (bio-oil) can help in restoring the ductility of an aged (brittle) asphalts by "re-dissolve" the assempled structures of asphaltenes.

Repercussions: (i) This study can pave the way for the substitution of high-cost carbonbased nanoparticles like fullerenes, nanotubes and graphenes with the much less expensive char from pyrolysis; (ii) the regeneration of aged asphalts by bio-oil reduces the production of new bitumen and the landfilling of aged ones.

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# Keywords

Char Pyrolysis wastes disposal bitumens

### Last published paper details

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#### Full title of article

The efficiency of bio-char as bitumen modifier

#### Journal

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#### All authors

V. Loise, P. Calandra, A. Policchio, L. Madeo, C. Oliviero Rossi, M. Porto, A. Abe, R. Agostino, P. Caputo

# **P.192** Green reinforcement of plastic packaging by starch addition: A coupled computational and experimental study

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# Abstract

Poly Lactic Acid (PLA) / Poly Butylene Adipate-co-

Terephthalate (PBAT) blends are used as packaging green materials since they constitute hydrophilic and biodegradable plastic. With the aim of improving the mechanical characteristics

of PLA/PBAT blends as biodegradable packaging materials for food products the addition of starch has been considered. In silico study performed by classical molecular dynamics (MD) highlighted that the addition of starch can reinforce the polymeric structure via starch-polymer interactions, suggesting that starch can be a suitable material to be added to the PLA/PBAT blend to obtain more resistant packaging materials. A snapshot of the MD simulation is reported in Fig. 1 left panel.

Experimental analysis of the mechanical properties of PLA/PBAT blends containing different amounts of starch confirmed what foreseen by MD, highlighting increases in Young modulus and glass transition as a function of added starch. Starch amount of 10 wt% turned out to be the optimum to maximize the elongation bearable under tensile stress before rupture (Fig. 1 right panel). The coupled theoretical/experimental approach constitutes added value of the present work, furnishing important data on the reinforcement of the packaging material performances and a molecule-based interpretation and comprehension of the observed phenomenon