

7<sup>th</sup> International Conference on  
**Materials Science & Nanotechnology**

July 15-16, 2024 at Vienna, Austria (*Hybrid Event*)



**Venue:** Hotel NH Danube City **Address:** Wagramer Str. 21, 1220 Wien, Austria

**Website URL:** [jamesmichael@materials-science.org](mailto:jamesmichael@materials-science.org)

**Email:** <https://materials-science.org/>



## Day - 01

## Day - 01

Monday, July 15 *(In-person)*

Monday, July 15 *(Virtual)*

**Hall Name: Stefan Zweig + Theodor Herzl**

Registrations - 08:00 - 08:50

(Time Zone - CEST)

Keynote presentations - 09:00-10:30

Timings-12:00 - 16:40

Morning Session-10:50 - 13:10

Through ZOOM

Afternoon Session- 14:00 -16:20

Evening Session-16:30 -18:30

## Day - 02

## Day - 02

Tuesday, July 16 *(In-person)*

Tuesday, July 16 *(Virtual)*

**Hall Name: Stefan Zweig + Theodor Herzl**

Keynote presentations - 9:00 -10:00

(Time Zone - CEST)

Morning session-10:00 -12:55

Timings: 10:00 - 17-15

Posters Presentations -13:40 -14:30

Through ZOOM

Afternoon Session - 14:30 -17:00

Day  
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MONDAY

# 7<sup>th</sup> International Conference on Materials Science & Nanotechnology

July 15-16, 2024 at Vienna, Austria (Hybrid Event)

Meeting Hall: Stefan Zweig + Theodor Herzl

Moderator: Clémence Delmas, *University of Lorraine, France*

08:00-08:50 Registrations

08:50-09:00 Opening Ceremony & Moderator Speech

## Keynote Session

09:00-09:30 ----- Title: Laser Shock Processing: An Emerging Technique for the Improvement of the Mechanical Behaviour and In-Service Performance of High-Added-Value Metallic Alloys

José Luis OCAÑA, *Universidad Politécnica de Madrid, Spain*

09:30-10:00 ----- Title: n-type semiconducting biomaterials

Mikio Fukuhara, *Tohoku University, Japan*

10:00-10:30 ----- Title: Quantized transport and tunable chiral conduction in topological magnets

Lia Krusin-Elbaum, *The City College of New York - CUNY, New York, NY, USA*

Group Photo & Refreshment Break (10:30-10:50)

## Technical Session: I

Session Chairs: *José Luis Ocaña & Debes Bhattacharyya*

10:50-11:10 ----- Title: Mechanical surface characterization 2.0 – what else can you do with a modern nanoindenter

Thomas Chudoba, *ASMEC GmbH, Germany*

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- 11:10-11:30 ----- Title: Pencil graphite/polypyrrole and pencil graphite/polypyrrole-Mn oxide electrodes for supercapacitors  
Murside Hacıismailoglu, *Bursa Uludag University, Turkey*
- 11:30-11:50 ----- Title: Enhancing the Pore Structure of Metal-Organic Frameworks for Improved Water treatment Efficiency  
Shaghayegh Naghdi, *Technische Universität Wien, Austria*
- 11:50-12:10 ----- Title: Poly(diallylmethylammonium) proton conducting membranes with high ionic conductivity at intermediate temperatures  
Aurélie Guéguen, *Toyota Motor Europe, Belgium*
- 12:10-12:30 ----- Title: The design of materials related to Lithium-ion batteries through theoretical studies  
Jyh-Chiang Jiang, *National Taiwan University of Science and Technology, Taiwan*
- 12:30-12:50 ----- Title: The recent advance in synthesis and applications of Magnéli phase titanium oxides  
Xiaoping Wu, *Chengdu Advanced Metallic Materials Industry Technology Research institute Co., Ltd, China*
- 12:50-13:10 ----- Title: Fatigue life improvement and residual stress retention of single crystal nickel CMSX-4® superalloy after corrosion and thermal exposure  
Jochen Fuhr & Lloyd Hackel, *Curtiss-Wright Surface Technologies., United States*

Lunch Break @ Restaurant (13:10-14:00)

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## Technical Session: II

Session Chairs: *Thomas Chudoba & Lia Krusin-Elbaum*

- 14:00-14:20 ----- Title: Design and characterization of based chitosan sol-gel films for textile substrates  
*Rosa Taurino, University of Florence, Italy*
- 14:20-14:40 ----- Title: Structural and electrical properties of NiO thin films on nanoporous Si fabricated by reactive DC sputtering  
*M. Cuneyt Hacıismailoglu, Bursa Uludag University, Turkey*
- 14:40-15:00 ----- Title: Functional Ordered Nanoporous Materials Derived from Nanostructured Block Copolymers  
*Daniel Grande, Institut Charles Sadron, France*
- 15:00-15:20 ----- Title: Study of Flexible ZnSnO-channel-based Thin Film Transistors  
*Kao-Shuo Chang, National Cheng Kung University, Taiwan*
- 15:20-15:40 ----- Title: High-performance van der Waals antiferroelectric  $\text{CuCrP}_2\text{S}_6$ -based memristors  
*Xixiang Zhang, King Abdullah University of Science and Technology, Saudi Arabia*
- 15:40-16:00 ----- Title: Carbon materials for solar steam-generation  
*Masahiro Toyoda, Oita University, Japan*
- 16:00-16:20 ----- Title: Promoting Sustainability Through New Advances In The Production Of Lithium-Ion Batteries As Part Of The Batwoman Project  
*Bernd Eschelmüller, AIT Austrian Institute of Technology GmbH, Austria*

Refreshment Break (16:20-16:30)

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- 16:30-16:50 ----- Title: **Hot Rolling of Ta-B and Ta-Al-B(B4C) Reactive Blends**
- Akaki Peikrishvili, Ferdinand Tavadze Institute of Metallurgy and Materials Science, Georgia*
- 16:50-17:10 ----- Title: **High-entropy alloys with excellent mechanical properties and irradiation resistance**
- Haiming Wen, Missouri University of Science and Technology, United States*
- 17:10-17:30 ----- Title: **Modulation of electrical, acoustic and optical properties of phthalocyanines by gas adsorption: interest for gas sensors development.**
- Jérôme BRUNET, Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, France*
- 17:30-17:50 ----- Title: **Essential oil-loaded coaxial wet-spun fibers for wound healing applications**
- Catarina S. Miranda, Centre for Textile Science and Technology (2C2T), University of Minho, Portugal*
- 17:50-18:10 ----- Title: **Synthesis and Stabilization of Metal Nanoparticles via Reactive High-Energy Ball Milling Passivated with Organic Ligands**
- Julie P. Vanegas, University of Texas Rio Grande Valley, Edinburg, Texas, United States*
- 18:10-18:30 ----- Title: **Fe and Sr co-doped  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  garnet-type solid state electrolyte: synthesis, structure and electrochemical properties**
- Anjan Sil, Indian Institute of Technology Roorkee, India*

Day-1 Concludes





**Day  
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TUESDAY

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Moderator: Hatice Ceylan Koydemir, *Texas A&M University, United States*

## Keynote Session

09:00-09:30 ----- Title: **Advanced Handheld Spectroscopic Eye-Safe Technology for Point-Of-Care Detection of Traumatic Brain Injury**

**Pola Goldberg Oppenheimer**, *University of Birmingham, United Kingdom*

09:30-10:00 ----- Title: **Protein interaction analysis by surface plasmon resonance and application**

**Dennis G. Drescher**, *Wayne State University, United States*

## Technical Session: III

**Session Chairs: Akaki Peikrishvili & Dennis G. Drescher**

10:00-10:20 ----- Title: **Flame retardant chicken feather/polypropylene composites – a novel approach towards efficacy improvement with improved feasibility**

**Debes Bhattacharyya**, *University of Auckland, New Zealand*

10:20-10:40 ----- Title: **High-Performance Air-Stable Solar Selective Absorber for CSP Applications up to 450 °C**

**Meryem Farchado**, *CIEMAT-PSA. Materials for Concentrating Solar Thermal Technologies Unit., Spain*

## Refreshment Break (10:40-10:55)

10:55-11:15 ----- Title: **Active Control of Springback Effect in Deep Drawing Processes: Theory and Experiment**

**Mostafa Mehrabi**, *University of Detroit Mercy, United States*

11:15-11:35 ----- Title: **Hall-Petch Equation: a possible modification for submicron-grained metals**

**NGUYEN Quang Chinh**, *Eötvös Loránd University, Hungary*

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- 11:35-11:55 ----- Title: Fabrication of 3D printed devices coated with thiol-grafted iron-based metal organic framework for heavy metal removal
- Daniel Roberto Sáenz Garcia, *Advanced Materials Research Center, (CIMAV) S.C., Mexico*
- 11:55-12:15 ----- Title: Spin-polarized electronic states of high- $T_c$  cuprate superconductors
- Hideaki Iwasawa, *National Institutes for Quantum Science and Technology (QST), Japan*
- 12:15-12:35 ----- Title: A nano-in-micro strategy to tackle the burden of pulmonary fungal diseases
- Filipa Sousa, *UCIBIO-REQUIMTE, Laboratory of Pharmaceutical Technology, Department of Drug Sciences, Faculty of Pharmacy University of Porto, Portugal*
- 12:35-12:55 ----- Title: Magneto-plasmonic nanoparticles for non-toxic biomarker detection
- Yevhenii Morozov, *AIT-Austrian Institute of Technology, Austria*

Lunch Break @ Restaurant (12:55-13:40)

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## Poster Presentations (13:40-14:30)

Poster Judges: *Pola Goldberg Oppenheimer & Akaki Peikrishvili*

- ICMSN-I ----- Title: **The Study of Sintered Wick Structure of Heat Pipes with Excellent Heat Transfer Capabilities**  
*Yong Sik, AHN, Pukyong National University, South Korea*
- ICMSN-II ----- Title: **Au(I)-TADF Emitters for High Efficiency Full-Color Vacuum-Deposited OLEDs and TADF-Sensitized Fluorescent OLEDs with Ultra high Brightness and Prolonged Operational Lifetime**  
*Gang Cheng, The University of Hong Kong, Hong Kong*
- ICMSN-III ----- Title: **The large pore-size characteristics on the electric double-layer capacitance for high voltage by <sup>19</sup>F-NMR: A quantitative evaluation**  
*Joo-il Park, Hanbat National University, South Korea*
- ICMSN-IV ----- Title: **Cooling Crystallization of L-Glutamic Acid for Crystalline control**  
*Jong Beom Lee, Hanbat National University, South Korea*
- ICMSN-V ----- Title: **Physical restoration of waste artificial graphite through heat treatment and recycling as an anode material for secondary batteries**  
*Yu-Jin Kim, Hanbat National University, South Korea*
- ICMSN-VI ----- Title: **Improving Bee Living Conditions through Composite Ecological Thermal Insulation**  
*Krystyna Wrześniewska-Tosik & Justyna Wietecha, LUKASIEWICZ Research Network- Lodz Institute of Technology, Lodz, Poland*
- ICMSN-VII ----- Title: **ZnO Transistors Fabricated by Atomic Layer Deposition Process at Low Temperature**  
*Dedong Han, Peking University, China*
- ICMSN-VIII ----- Title: **Durable Triboelectric Nanogenerator on Coiled Head of Acupuncture Needle**  
*Saira Iqbal, City University of Hong Kong, Hong Kong*

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ICMSN-IX ----- Title: Temperature dependent phase transformation in Ag-SiO<sub>2</sub>-TiO<sub>2</sub> nanocomposites for multifunctional layer on Ni-Ti memory shape alloy  
Jacek Podwórny, Łukasiewicz Research Network-Institute of Ceramics and Building Materials

## Award Ceremony

## Technical Session: IV

Session Chairs: NGUYEN Quang Chinh & Mostafa Mehrabi

14:30-14:50 ----- Title: Identifying a critical nucleus for ice nucleation on hydrophilic and hydrophobic surfaces

Nan Yao, Princeton University, United States

14:50-15:10 ----- Title: Low-cost point of care technology for personalized medicine

Hatice Ceylan Koydemir, Texas A&M University, United States

15:10-15:30 ----- Title: Development of intelligent particles to prevent dental caries

Peter Zilm, The University of Adelaide, Australia

15:30-15:50 ----- Title: Intranasal administration of Pt(IV)-Based nanostructured coordination polymers for glioblastoma therapy

Fernando Novio, Universitat Autònoma de Barcelona, Spain

## Refreshment Break (15:50-16:00)

16:00-16:20 ----- Title: A Comprehensive study of Gum Arabic/Chitosan Polyelectrolyte Complexes

Clémence Delmas, University of Lorraine, France

16:20-16:40 ----- Title: The structure and properties of the high temperature recovered nanoscale carbon

Akaki Peikrishvili, Ferdinand Tavadze Institute of Metallurgy and Materials Science, Georgia

16:40-17:00 ----- Title: Development of 3D-printed breast cancer models for the evaluation of anticancerous systems

David Limón Magaña, NOVA School of Science and Technology, Portugal

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17:00-17:20 -----

Title: Preparation and characterization of multifunctional Ag-SiO<sup>2</sup>-TiO<sup>2</sup> nanocoatings on NiTi SMA

*Karolina Dudek, Łukasiewicz Research Network-Institute of Ceramics and Building Materials, Poland*

**Day-2 Concludes**

# Virtual Scientific Program



Join Zoom Meeting



Meeting ID: 836 2276 7552

Passcode: 741813

Day  
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MONDAY

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July 15-16, 2024 at Vienna, Austria (Hybrid Event)

Time Zone: Central European Summer Time (CEST)

## Virtual Presentations Through ZOOM

- 12:00-12:20 ----- Title: An automated and accelerated computational framework to compute finite temperature properties including anharmonic effects in different property domains  
*Pinku Nath, Hokkaido University, Japan*
- 12:20-12:40 ----- Title: Atomic-scale cognition of c-Si/a-Si:H interface in high efficiency silicon heterojunction solar cells  
(Keynote)  
*Kun ZHENG, Beijing University of Technology, China*
- 12:40-13:00 ----- Title: Capacitive Piezotronic Force Sensor with Ultra-Low Power for Next-Generation Sensory Memory System  
*Chao-Hung Wang, Miin Wu School of Computing, National Cheng Kung University, Taiwan*
- 13:00-13:20 ----- Title: Development of automotive quality high-strength steel microalloying principles to reduce production costs with keeping required mechanical performance  
*Aleksei Dagman, Novolipetsk Steel (NLMK), Russia*
- 13:20-13:40 ----- Title: Toroidal topology and its manipulation in ferroelectric polymers  
*Mengfan Guo, University of Cambridge, United Kingdom*
- 13:40-14:00 ----- Title: Addressing Midwakh and E-cigarette use in the Gulf region  
*Sarah Dalibalta, American University of Sharjah, UAE*
- 14:00-14:20 ----- Title: Chitosan- and graphene oxide-based composites for the adsorption of caesium, cobalt and europium from aqueous solution  
*Galina Lujaniene, Center for Physical Sciences and Technology (FTMC), Lithuania*
- 14:20-14:40 ----- Title: Properties of Mesoporous Silicon (MSMPs) as a new adjuvant in the formulation of vaccine complexes  
*Manuel Gómez Del Moral, Complutense University, Facultad De Medicina-UCM, Spain*

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- 14:40-15:00 ----- Title: Novel potentiometric sensors for continuous metabolite monitoring  
Idan Tamir, *QuLab Medical Ltd, Israel*
- 15:00-15:20 ----- Title: Rashba metasurfaces – strain-tuned surface states towards perfect darkness  
Anna Kusmartseva, *Loughborough University, United Kingdom*
- 15:20-15:40 ----- Title: Preliminary Study of Wound Oxygenation Comparing Skin Substitutes and Dressings  
Linwood R. Haith, Jr, MD, *Drexel University, USA*
- 15:40-16:00 ----- Title: Synthesis and Characterization of  $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$  and  $\text{La}_2\text{NiTiO}_6$  Double Perovskite Nanoparticles  
Pablo Vinicio Tuza Alvarado, *Universidad Técnica de Ambato, Ecuador*
- 16:00-16:20 ----- Title: Utilize pMAIRS to Evaluate the Conformation and Orientation of  $\alpha$ -Synuclein(61-95) in Monolayer at Interface with Residue Level Resolution  
Chengshan Wang, *Middle Tennessee State University, USA*
- 16:20-16:40 ----- Title: Effect of polarization on Nb and Mn doped  $\text{BaTiO}_3$  ferroelectric on its photovoltaic, electrical and electrical properties  
Jesús Iván Peña Flores, *Centro de Investigación y de Estudios Avanzados del IPN - CINVESTAV, Mexico*

Day-1 Concludes



Day  
2

TUESDAY

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- 10:00-10:20----- Title: Microscopic behavior of self-diffusion in liquid Sn and Pb using molecular dynamics simulation  
Masato Shiinoki, Waseda University, Japan
- 10:20-10:40----- Title: Tumor microenvironment targeting for glioblastoma multiforme treatment via hybrid cell membrane coating supramolecular micelles  
Xiaobei Huang, Chinese Academy of Sciences, China
- 10:40-11:00----- Title: CO<sub>2</sub> permeation on Zn<sup>2+</sup> modified Al<sub>2</sub>O<sub>3</sub>-carbonate membranes  
Liu Qu, Shenyang Ligong University, China
- 11:00-11:20----- Title: Effects Of Dietary Solvents on Microhardness and Inorganic Elemental Composition of Computer-Assisted Design/Computer-Assisted Manufacturing Dental Composites  
Selva Malar Munusamy, Universiti Malaya, Malaysia
- 11:20-11:40----- Title: Mechanical stability of carbon/ramie fiber hybrid composites under hygrothermal aging  
Ming Cai, Shanghai University of Engineering Science, China
- 11:40-12:00----- Title: Approaches to the design of efficient and stable catalysts for biofuel reforming into syngas: Doping the mesoporous MgAl<sub>2</sub>O<sub>4</sub> support with transition metal cations  
Vladislav A. Sadykov, Federal Research Center Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia
- 12:00-12:20----- Title: Spectroscopic ellipsometry and B-spline coefficients of non-hydrogenated amorphous silicon for amorphous silicon based semiconductors  
M. A. Ebdah, King Saud University, Saudi Arabia
- 12:20-12:40----- Title: Specific and label-free biosensing with a novel biologicaly-modified field-effect transistor (BioFET)  
Gil Shalev, Ben-Gurion University of the Negev, Israel
- 12:40-13:00----- Title: Self-Healing Silsesquioxane-Based Materials  
Anna Kowalewska, Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Poland

Day  
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- 13:00-13:20----- Title: The dominance of pretransitional effects in liquid crystal based nanocolloids: MBBA with transverse and 5CB with the longitudinal permanent dipole moment plus BaTiO<sub>3</sub> nanoparticles  
**Sylwester J Rzoska**, *Institute of High Pressure Physics Polish Academy of Sciences, Warsaw, Poland*
- 13:20-13:40----- Title: Polycatenanes Formed of Self-Assembled Metal Organic Cages  
**Antonino Famulari**, *Politecnico di Milano, Milan, Italy*
- 13:40-14:00----- Title: Unique features of mRNA-LNP Covid-19 vaccine nanoparticles explaining the acute adverse effects and post-vaccine syndrome  
**Janos Szebeni**, *Semmelweis University, Institute of Translational Medicine, Hungary*
- 14:00-14:20----- Title: Safer and sustainable plastic materials by toxicity screening  
**Peter Behnisch**, *BioDetection Systems, Netherlands*
- 14:20-14:40----- Title: From coffee to green roads: a sustainable recycling of silver-skin coffee wastes  
**Cesare Oliviero Rossi**, *University of Calabria CTC, Italy*
- 14:40-15:00----- Title: Hierarchical self-organization of Janus Nanoparticles and polymersomes for bio-applications  
**Voichita Mihali**, *University of Basel, Switzerland*
- 15:00-15:20----- Title: Synthesis, characterization and applications of rod-coil block copolymer:fullerene water-processable nanoparticles  
**Anna Maria Ferretti**, *Istituto di scienze tecnologie chimiche "Giulio Natta" SCITEC-CNR, Italy*
- 15:20-15:35----- Title: Synthetic strategies for composite materials formed by Magnetic Nanoparticles (MNPs) and Metal Organic Frameworks (MOFs)  
**Yaiza Martín García**, *University of La Laguna, Spain*  
(Poster Presentation)
- 15:35-15:55----- Title: An alternative to photodynamic therapy via graphene-doped quantum dots  
**Paulo Cesar De Moraes**, *Catholic University of Brasilia, Brazil*  
(Keynote)

**Day  
2**

TUESDAY

# 7<sup>th</sup> International Conference on **Materials Science & Nanotechnology**

**July 15-16, 2024 at Vienna, Austria (Hybrid Event)**

- 15:55-16:15----- **Title: Effect of Thermocycling on the Flexure Strength of 3D-Printed Denture Materials**  
*Rui Li, University at Buffalo, USA*
- 16:15-16:35----- **Title: Phase change ultrasound contrast agents: new method, new opportunities**  
*Caroline de Gracia Lux, University of Texas Southwestern Medical Center, USA*
- 16:35-16:55----- **Title: Outstanding Hardening Effect of High-Temperature Aging of Alloy Ti-6Al-4V Composite Reinforced with TiC**  
*Sergey Prikhodko, University of California Los Angeles, USA*
- 16:55-17:15----- **Title: Measuring Dynamic Diffraction in HREM Images**  
*Rodney Herring, University of Victoria, Canada*

**Closing Ceremony**

*Keynote Talks*  
**DAY-1**

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**Laser Shock Processing: An Emerging Technique for the Improvement of the Mechanical Behaviour and In-Service Performance of High-Added-Value Metallic Alloys**

J.L. Ocaña, I. Angulo, W. Warzanskyj, F. Cordovilla, A. García-Beltrán, J.A. Porro, M. Díaz

*UPM Laser Centre and ETSI Industriales. Polytechnical University of Madrid. C/ José Gutiérrez Abascal, 2. E-28006 Madrid. Spain*

Profiting by the increasing availability of laser sources delivering intensities in the GW/cm<sup>2</sup> range and with pulse energies in the range of several Joules, Laser Shock Processing (LSP) is consolidating as an effective technology for the improvement of mechanical properties and in-service behaviour of high-added-value metallic alloys and is being developed as a practical process amenable to production engineering. The main acknowledged advantage of the LSP technique consists on its capability of inducing a relatively deep compression residual stresses field into metallic alloy pieces allowing such improved mechanical behaviour.

Following a short description physical foundations of the technique, the set of theoretical/computational methods developed by the authors for the predictive assessment and experimental implementation of LSP treatments will be presented, Subsequently, the experimental facilities used at the UPM for the practical implementation of LSP processes will be presented and some representative results on the residual stress profiles and associated properties modification successfully reached in typical materials (specifically Al and Ti alloys) under different LSP irradiation conditions will be referred.

It is expected that the presentation of the LSP technique serves as a fruitful and enlightening starting point for the development of new research on the improvement of the in-service behaviour of critical metallic components (as, i.e. in the energy, aerospace and biomedical fields).

**Biography:**

Prof. Dr. Ing. José L. Ocaña is MSc. (1979) and PhD. (1982) in Industrial Engineering (Energy) at the Polytechnical University of Madrid (Spain). Chair Professor of Mechanical Engineering at the ETSII-UPM School of Engineering and Founder Director of the UPM Laser Centre at this University.

He has actively promoted and participated in national (Spain) and worldwide R&D initiatives in the field of scientific and industrial applications of high power lasers, especially in high intensity laser-matter interaction, laser surface treatments, laser micromachining and on-line monitoring and control of industrial laser applications. As a result, he is author/coauthor of more than 250 scientific papers and more than 300 communications in the field of laser technology and applications.

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### **n-type semiconducting biomaterials**

**Mikio Fukuhara, Tomonori Yokotsuka, Tetsuo Samoto and Toshiyuki Hashida**  
*New Industry Creation Hatchery Center (NICHe), Tohoku University, Japan*

There has been no research conducted thus far on the semiconducting behavior of biomaterials. Cellulose and chitosan are the first and second most produced natural compounds on Earth, and their molecular structures are very similar. In this study, we present n-type semiconducting biomaterials composed of amorphous kenaf cellulose fiber (AKCF)<sup>1</sup> and chitosan nanofiber (AChNF)<sup>2</sup> papers with a rectification effect and a voltage-controlled N-type negative resistance. The AKCF and AChNF generate an alternating-current (AC) waves with frequencies of 40.6 and 7.8 MHz from a direct-current (DC) voltage source at its threshold voltage (electric field of 187 and 5.26 kV/m), which is accompanied by a switching effect with four and third -order resistance changes at 298 K, respectively. This effect is attributed to the voltage-induced occurrence of strong field domains (electric double layers) at the cathode and depletion at the anode of the both devices, based on the dynamics of a collective proton-relay along the hybrid-hydrogen-bonded one-dimensional chain. Electron spin resonance spectral analyses showed that conducting electrons of KCNF and ChNF were identified as radicals on the alkoxy group C-O• and aminyl N•-H radicals, respectively. The AChNF also showed energy storage properties of 694.4 mJ/cm<sup>2</sup>. The light and flexible cellulose (or chitosan) -semiconductors may open up new avenues in soft electronics such as switching effect devices and bio-sensors, primarily as they are composed of renewable natural compounds. Hall effect measurements<sup>3</sup> indicate an n-type semiconductor with a mobility of 10.66 cm<sup>2</sup>/Vs.

<sup>1</sup> M. Fukuhara *et al. Sci. Rep.***12**, 21899 (2022).

<sup>2</sup> M. Fukuhara *et al. AIP Adv.***14**, 035103 (2024).

<sup>3</sup> M. Fukuhara *et al. Sci. Rep.***14**, 8692 (2024).

### **Biography:**

Dr. Fukuhara received PhD from Osaka University in 1979, worked for a Japanese company, and then started to research of electronics of amorphous materials as an associate professor in 2006 and as a visiting professor in 2014 at Tohoku University. He became a Research Fellow after retiring from NICHe in 2018, and currently continues to research of bioelectronics as Senior Research Fellow. He studied abroad at Pennsylvania State University in the United States for research on piezoelectric materials and superconductivity from 1987 to 1989, as senior visiting scientist.

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**Quantized transport and tunable chiral conduction in topological magnets**

**Lia Krusin-Elbaum**

*The City College of New York - CUNY, New York, NY, USA*

Current realizations of quantized anomalous Hall (QAH) and axion insulator states in magnetic topological insulators, featuring dissipation-free chiral edge currents, make it apparent that when magnetism and band topology combine the emergent electron and spin behaviors open a path to chirality-based implementations in future quantum devices. We have recently discovered a new Berry-curvature-driven QAH regime at higher temperatures [1] in the Mn(Bi,Sb)<sub>2</sub>Te<sub>4</sub> class of van der Waals intrinsic topological magnets (ITM), where Mn ions self-organize into a superlattice of Mn monolayers that can be separated on-demand. Robust ferromagnetism of such superlattice opens up a large surface gap, and QAH conductance reaches an  $e^2/h$  quantization plateau, even in the presence of the bulk states. The demanding tunability of the bandstructure and exchange interactions in these materials pose significant challenges in accessing chiral channels and the quantized transport regime. In this talk I will describe our new tuning technique for accessing topological surface currents towards realizing QAH [2] and our most recent results on achieving bandstructure-tunable chiral conduction in the Weyl topological magnet MnSb<sub>2</sub>Te<sub>4</sub> with a reversible intake and release of ionic hydrogen [3]. Further, our manipulation of topological Weyl bands led us to the discovery of unusual in-plane-field quantized Hall transport, showcasing a scalable strategy to manipulate chiral channels for chiral logic and topological spintronics. \*Supported by NSF grants DMR-2011738 and HRD-2112550.

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**Biography:**

Lia Krusin-Elbaum is a Professor of Physics at The City College of New York since 2010. her Ph.D. degree is in Condensed Matter Physics (NYU, 1979) and she was a scientist at the IBM's T.J. Watson Research Center, NY (1979-2010). Dr. Krusin-Elbaum is a recipient of ten IBM Invention Achievement Awards and holds over 27 US patents. She is a Fellow of the American Physical Society (1993-) and was elected (2022) to serve on the USDOE Basic Energy Sciences Advisory Committee. She is a co-lead of the Columbia U. NSF-MRSEC PAQM (2020-) and of the NSF-CREST IDEALS Centers (2015-).

*Scientific Session*

**DAY-1**



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## **Mechanical surface characterization 2.0 – what else can you do with a modern nanoindenter**

**Thomas Chudoba**  
*ASMEC GmbH, Dresden, Germany*

Many different test methods are used for the mechanical characterization of surfaces and coatings. Nevertheless, it is often not possible to achieve a good correlation between test results in the laboratory and the behavior of components in an application. The reason for that is the incomplete knowledge of the real application conditions and the difference to the test conditions. In real applications there exists mostly a combination of normal, lateral, torsional and dynamic forces.

In the talk it will be explained, how dynamic and lateral forces can be measured and considered in the analysis. The difference between quasi-static and dynamic hardness and modulus measurements is explained and the advantages of dynamic tests are illustrated. It will be further discussed how the dynamic capabilities can be used for fatigue tests and the measurement of rubber or polymers.

With a lateral force unit as second measuring head for nanoindenters it is possible to simulate lateral forces and displacement with high accuracy additionally to normal forces. This is a step closer to application conditions. In the talk it will be explained how the lateral force unit is working and which corrections are necessary. Further different analysis methods for lateral force-displacement curves will be introduced. This includes the analysis of many reciprocating cycles in micro wear tests, the determination of the lateral contact stiffness and a new method for the determination of the Poisson's ratio.

In a last part several methods for a mapping of mechanical surface properties will be explained. Such a mapping gives better access to the homogeneity of surfaces and to the distribution of components in a composite. The weakest points in a surface can be better found by a mapping than by a single row of indentations. Several mapping examples will be are given.

### **Biography:**

Career start in microelectronics for development of lithographic masks; PhD in Physics in the field of ion implantation and contact mechanics; 1997- 2002 Post Doc at TU Chemnitz, afterwards visiting scientist at BAM, EMPA and CSIRO; 2004 founding the own company ASMEC GmbH with the aim to develop and sell nanomechanical testers; at present convenor of working group 4 within ISO TC164 SC3 responsible for the revision of the indentation standard ISO 14577

## Pencil graphite/polypyrrole and pencil graphite/polypyrrole-Mn oxide electrodes for supercapacitors

Dilek Vatansever, **Murside Hacıismailoğlu** and Mursel Alper  
*University of Uludağ, Department of Physics, Bursa, Turkey*

Pencil graphite (PGE) was used as a current collector for the electrodeposited polypyrrole (PPy) layer and PPy-Mn oxide layer. The electrochemical, chemical and structural properties were studied as a function of monomer concentration and layer thickness for the PGE/PPy electrodes. The capacitive behavior was studied by cyclic voltammetry (CV) in an acidic solution. According to the characterizations, the convenient electrode was chosen and used for the electrodeposition of Mn-oxide on it. The aforementioned properties of these PGE/PPy-Mn oxide electrodes were investigated depending on the Mn ion concentration and deposition charge density. The capacitive behavior was studied by CV in an acidic solution as well. For the PGE/PPy electrode, the highest specific capacitance was calculated as 695 F/g, and the stability was obtained as 77% after 1000 times cycled. For the PGE/PPy-Mn oxide electrode the highest specific capacitance was calculated as 394 F/g, and the stability was obtained as 90% after 1000 times cycled. The results show that the Mn-oxide particles cause to decrease in the specific capacitance but increase the stability significantly. From those high-valued electrodes, symmetrical and asymmetrical supercapacitors were fabricated. Fig. 1 (a) shows the CV curves at the scan rate of 50 mV/s for symmetrical and asymmetrical supercapacitors. The power density was calculated as 119 W/kg from the CV curves obtained at the scan rate of 2 mV/s for these devices. They both could enlighten an LED as given in Fig. 1 (b and c). Such supercapacitors can be used in the devices working at low-medium power density.



Figure 1. (a) CV curves of the symmetrical and asymmetrical supercapacitors, (b) symmetrical and (c) asymmetrical supercapacitors enlighten an LED.

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**Biography:**

Murside Haciismailoglu received a Ph.D. degree in solid-state physics from Bursa Uludag University, Bursa, Turkiye in 2010. She worked as a post-doctoral researcher at the Department of Physics in the University of Bristol, U.K., in 2012. She is currently with the Department of Physics, Bursa Uludag University as an associate professor. She is active in the fields of materials used in supercapacitor applications, and magnetic materials and their magnetotransport properties.

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## Enhancing the Pore Structure of Metal-Organic Frameworks for Improved Water Treatment Efficiency

Shaghayegh Naghdi<sup>1</sup>, Mohammad Zendeabad<sup>2</sup>, Pablo Ayala<sup>1</sup>, Alexey Cherevan<sup>1</sup>, Rémy Guillet-Nicolas<sup>3</sup>, Santu Biswas<sup>4</sup>, Thomas Haunold<sup>1</sup>, Günther Rupprechter<sup>1</sup>, Maytal C. Toroker<sup>4</sup>, Freddy Kleitz<sup>3</sup>, Dominik Eder<sup>1</sup>

<sup>1</sup> Department of Material Chemistry, Technische Universität Wien, 1060 Vienna, Austria

<sup>2</sup> Department of Water, Atmosphere, and Environment, University of Natural Resources and Life Sciences Vienna, Austria

<sup>3</sup> Department of Inorganic Chemistry- Functional Materials, Faculty of Chemistry, Universität Wien

<sup>4</sup> Technion - Israel Institute of Technology, Haifa 3600003, Israel.

In the realm of environmental and energy technologies, Metal-Organic Frameworks (MOFs) have gained significant attention due to their unique blend of customizable light-harvesting, catalytic functionalities, and remarkable adsorption capabilities. Acknowledging the challenges posed by the limited micropores of MOFs in fluid dynamics, particularly regarding reactant diffusion, we have pioneered an innovative approach. This entails introducing mesopores into mixed-ligand MOFs through selective ligand removal (SeLiRe) via thermolysis.

Our methodology has resulted in the development of a series of MOFs within the MIL-125-Ti family, featuring dual hierarchical pore architectures: cavity-type pores and fracture-type pores. Notably, these tailored pore structures have elevated Hydrogen Evolution Reaction (HER) rates by up to 400%, representing a groundbreaking advancement in designing hierarchical MOFs with enhanced functionality in liquid environments [1].

Furthermore, our research delved into the impact of selective ligand removal on the adsorption properties of MOFs, with a focus on purifying water from organic pollutants. The presence of unsaturated metal sites, coupled with improved accessibility facilitated by SeLiRe, significantly enhanced adsorption efficiency. In fact, these modified MOFs exhibited adsorption rates up to 4 times greater than those of untreated MOFs [2].

Taking a significant leap forward, we introduce two novel mixed-coordination Cu-based MOFs, labeled TUW-1 and TUW-2. These have been synthesized as superior adsorbents for highly efficient nitrate removal from both water and real wastewater samples. Notably, these MOFs demonstrate exceptional stability in aqueous conditions (for over 365 days). Additionally, both MOFs exhibit rapid adsorption kinetics and unprecedented nitrate adsorption capacities, surpassing all known adsorbents, even under neutral pH levels. These findings underscore the potential of MOFs as promising materials for effective and sustainable water purification.

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**Biography:**

Dr. Shaghayegh Naghdi is a postdoctoral researcher at TU Wien, where she has been the MOFs area leader in the molecular material chemistry group since May 2022. her current research is centered on designing and applying metal-organic frameworks in environmental efforts, specifically in photocatalysis and water treatment. In April 2022, she completed her Ph.D. in natural sciences at TU Wien, focusing on designing new MOFs for hydrogen evolution (HER) and synthesizing new water-stable MOFs. Before joining academia, she spent five years in the industry. She earned her master's degree in organic chemistry from Kharazmi University in Tehran in 2008.

## **Poly(diallylmethylammonium) proton conducting membranes with high ionic conductivity at intermediate temperatures**

Aurélie Guéguen, Antonela Gallastegui, Fabrizia Foglia, Paul F. McMillan, Nerea Casado, David Mecerreyes

Operating proton exchange fuel cells at high/intermediate temperature (~100-200 °C) is particular of interest for automotive applications as this will ease heat and water management while keeping good performance (higher CO tolerance, faster reaction kinetics, among others). Perfluorosulfonic acid membranes normally used at low temperature aren't suited for operation > ~100 °C due to poor thermal stability above that temperature and low proton conductivity under dry conditions. Current main type of high temperature membrane investigated is polybenzimidazole (PBI) doped with H<sub>3</sub>PO<sub>4</sub> (PA). However, loss of PA from the PBI still need to be solved (1). High anhydrous proton conductivity (~10<sup>-2</sup>-10<sup>-3</sup> S/cm above 100°C) have been reported for protic ionic liquids (2). One way to incorporate them in the polymeric membrane is through direct polymerization, without the need of any solvent (3). For example, cationic poly(diallyldimethylammonium) (PDADMA) backbone in combination of different anions has shown superior mechanical and electrochemical properties (4, 5). We have expanded this family of poly(ionic liquid)s (6) by investigating protic poly(diallylmethylammonium), PDAMAH<sup>+</sup>X<sup>-</sup>, self-standing ionic polymers. The new membranes were synthesized by photopolymerization of new protic ionic liquids DAMAH<sup>+</sup>X<sup>-</sup> obtained by a simple one-step reaction between diallylmethylamine DAMA and several acids of different chemical nature. New protic ionic liquids and protic polymeric membranes were fully characterized (chemical composition, thermo-mechanical properties, ionic conductivity). Highest ionic conductivity was found for the protic polymeric membrane based on methane sulfonate anion, reaching a value of 2 10<sup>-3</sup>S/cm at 100 °C and dry conditions. Furthermore, Neutron Scattering studies (QENS) showed that the protic membranes can uptake water and retain part of it upon drying, which can be beneficial during fuel cell operation and help maintain proton conductivity.

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### **Biography:**

Aurélie Guéguen is a senior engineer at Toyota Motor Europe carrying R&D activities on materials for energy applications such as lithium batteries and proton exchange fuel cells. After getting a PhD from Michigan State University in the field of solid state chemistry, Aurélie changed her focus and investigated lithium batteries, first working on understanding degradation in Li-ion batteries before working on the challenging development of new material for solid state batteries, notably polymer electrolytes. Polymeric membranes are a fascinating family of materials. Some similarities between polymer electrolytes used in Li batteries and proton exchange membranes can inspire design of innovative proton exchange membranes.

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**The design of materials related to Lithium-ion batteries through theoretical studies**

Liang-Ting Wu, Shi-Hong Xu, Yu-Ting Zhan, Zhong-Lun Li, and **Jyh-Chiang Jiang\***

Lithium-ion batteries (LIBs) are widely used as a power source in various applications, such as energy storage and electronic devices. In recent years, Ni-rich layered lithium nickel-cobalt-manganese oxides (NCM) have been highlighted as advanced cathode materials for high-capacity LIBs. However, their low interfacial stability during cycling limited the cell's electrochemical performance. In addition, Extreme conditions, such as heat waves, cold snaps, deep seas, and high altitudes, markedly diminish the performance of lithium batteries. This results in low-capacity retention and safety concerns when these batteries are utilized in electric vehicles and energy storage stations (Nature 529, 515–518 (2016)). In my talk, I will introduce the first-principles density functional theory calculations to systematically investigate surface instabilities of NCM811 ( $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ ), including  $\text{O}_2$  formation and surface distortions, and explore the effect of doping, including S and Cl on structural stability. In addition, I will introduce our research using density functional theory (DFT) and real solvent class conductor screening model (COSMO-RS) to explore the liquid range of 190 binary mixtures. As well, we calculated the saturation solubility of LiTFSI salts to identify ideal mixtures with high solubility. The results showed high accuracy, making it suitable for early solvent evaluation.

**Biography:**

Jyh-Chiang Jiang graduated from National Taiwan University in 1986 with a B.S. in Chemistry and received his Ph.D. in Chemistry in 1994. After working as a postdoctoral fellow at IAMS, Dr. Jiang joined the National Taiwan University of Science and Technology (NTUST) faculty in 2001. He focuses on the theoretical and computational chemistry study of heterogeneous catalysis, optoelectronic materials, and Li-ion batteries. He has more than 220 papers in peer-reviewed journals. his research has also resulted in 4 patents. Dr. Jiang has been chairman of the Taiwan Theoretical and Computational Molecular Sciences Association from August 2019 to July 2023.

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**The recent advance in synthesis and applications of Magnéli phase titanium oxides**

Xiaoping Wu<sup>1</sup> & Haibo Wang<sup>2</sup>

<sup>1</sup>Chengdu Advanced Metallic Materials Industry Technology Research institute Co., Ltd, Chengdu, 610303, China

<sup>2</sup>Ansteel Research Institute of Vanadium & Titanium, Panzhihua, 617000, China

Magnéli phase titanium oxides ( $Ti_nO_{2n-1}$ ,  $4 < n < 9$ ) are electrically conducting ceramic materials. The synthesis and applications of those ceramic materials have recently attracted tremendous attention because of their applications in a number of existing and emerging areas. Magnéli phase titanium oxides are generally synthesized through the reduction of titanium dioxide using hydrogen, carbon, metals or metal hydrides as reduction agents. More recently, the synthesis of nanostructured titanium sub-oxides has been making progress through optimizing thermal reduction process or using more reactive titanium-containing precursors. Magnéli phase titanium oxides have attractive properties such as electrical conductivity, corrosion resistance and optical properties. Among Magnéli phase titanium oxides,  $Ti_4O_7$  has received the most widespread attention due to its excellent electrical conductivity, and chemical and electrochemical stability. Magnéli phase titanium oxides,  $Ti_4O_7$  in particular, have played important roles in a number of areas such as conducting materials, fuel cells, and organic degradation. Titanium sub-oxides also show promising applications in batteries, solar energy, coatings, and electronic and optoelectronic devices. In this talk, the recent progress in the synthesis methods and applications of Magnéli phase titanium oxides in the existing and emerging areas are highlighted and discussed.

**Biography:**

Dr Wu obtained B.Sc and M.Sc degrees in chemistry from universities in China and a PhD in chemistry from University of London, and had research experience in chemistry/material science in various universities and research organizations in UK and China. Dr Wu is currently a senior scientist in Chengdu Advanced Metallic Materials Industry Technology Research institute Co., Ltd.



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**Fatigue life improvement and residual stress retention of single crystal nickel CMSX-4® superalloy after corrosion and thermal exposure**

Nicolau I. Morar<sup>1\*</sup>, Noah Holtham<sup>2</sup>, **Lloyd Hackel**<sup>3\*</sup>, Keivan Davami<sup>2</sup>, Montu Sharma<sup>3</sup>, Adrian DeWald<sup>4</sup> and Rajkumar Roy<sup>1</sup>

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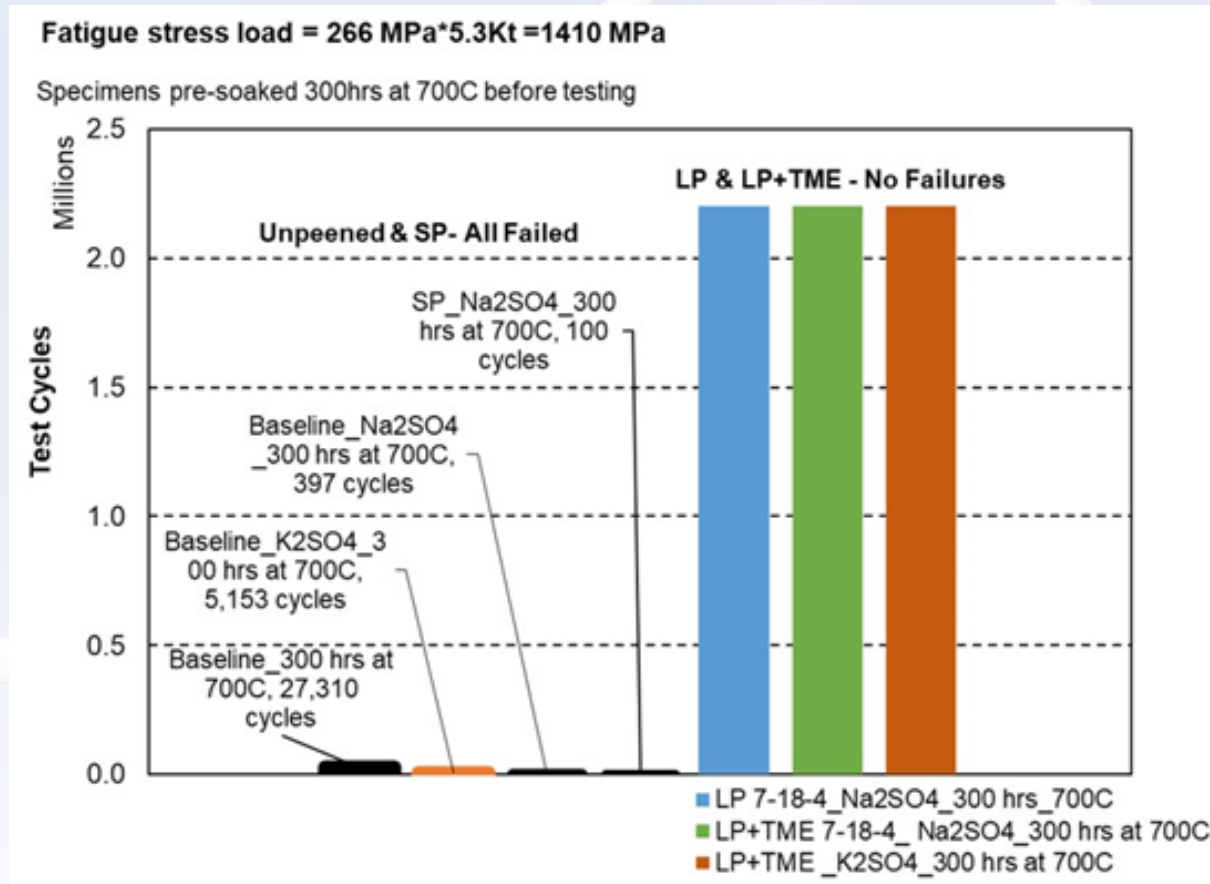
<sup>2</sup> University of Alabama, Department of Mechanical Engineering, Tuscaloosa, AL 35487,

United States

<sup>3</sup> Curtiss Wright Surface Technologies - Metal Improvement Company, United States

<sup>4</sup> Hill Engineering, LLC, United States

This study investigated fatigue life and strength and stress relaxation after thermal exposure and fatigue testing of laser peened, shot peened and un-peened specimens of single crystal (SX) nickel superalloy. Specimens were tested under fixed maximum load and 5 Hz cycle rate to 10% compliance failure after first painting with a sodium or potassium sulfate paste and thermal exposure at 700°C for 300 hours. Tests comparing un-peened, shot peened and laser peened specimens included a novel process in which laser peening was combined with a cyclic laser peening plus thermal microstructure engineering process (LP+TME) involving application of layers of laser peening using high energy and large spots combined with interspersed cyclic annealing. Residual stress (RS) measurements by the Slitting Technique showed the plastic penetration depth of laser peening exceeded shot peening by a factor of 24. Further, measurements of an LP+TME specimen showed 5 mm depth of retention of RS post hot-corrosion exposure and fatigue testing. Deep penetration of laser peening is easily explained by the large laser spot footprint of 5 mm compared to shot peening ball size of 0.5 mm as depth of plastic compression in any peening process is directly related to spot size on the surface. Somewhat surprising retention of RS after thermal exposure by the LP+TME process is being further investigated. Dramatic decrease in fatigue lifetimes resulted for un-peened and shot peened specimens when exposed to the corrosives at the 700°C and 300-hour time. In contrast three laser peened specimens all achieved multi-million-cycle runout without failure, indicating treatment by LP gives a statistically significant large benefit for fatigue life compared to all five non-laser peened samples. The chart below summarizes the fatigue test results. Additional tests with increased load showed fatigue strength improvement of 2:1 by laser peening. Clearly tests with greater sample count and potentially fatigue testing at high temperature are required. Tests are now continuing with a large quantity of test specimens using a 3rd generation SX superalloy, CMSX-4® Plus (SLS).



Fatigue life of notched four-point bending CMSX-4 nickel-based superalloy specimens left un-peened, treated by shot or laser peening then with pre-test thermal or chemical-plus-thermal exposure and finally fatigue tested as noted.

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**Design and characterization of based chitosan sol-gel films for textile substrates**

**Rosa Taurino**, Maria Cannio, Stefano Caporali, Stefano Martinuzzi, Emanuele Galvanetto, Francesca Borgioli, Dino Boccacini<sup>3</sup>

*Department of Industrial Engineering, University of Florence, Via di Santa Marta 3, Firenze, 50139, Italy  
National Interuniversity Consortium of Materials Science and Technology (INSTM), Via Giusti 9, Firenze, 50121, Italy*

This research aimed to develop an innovative textile finish using chitosan sol-gel coatings to imbue fabrics hydrophobic 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, vinyltrimethoxysilane (VTMS) was used as coupling agent. Various formulation of sol-gel hybrids loaded with different amounts of chitosan were prepared and applied onto different textile substrates (cotton 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, several characterizations have been performed to analysis the effect of film composition on several properties. Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) for microstructure examination, water contact angle measurements for surface wettability assessment, hydrolytic 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.

**Biography:**

Dr Rosa Taurino is research at the Department of Industrial Engineering (DIEF) and Professor of Materials Science and Technology at the University of Florence. Since 2005 the research activity is focused on the development of hybrid materials by sol-gel process (multifunctional coatings or reinforced polymer matrix by in situ silica generation), in the valorisation of waste; (industrial waste, and agro-waste) in new materials for the green-building sector (ceramic materials and composite materials) and in the development of new materials for 3D printing process.

## Structural and electrical properties of NiO thin films on nanoporous Si fabricated by reactive DC sputtering

M. Cunevt Haciismailoglu\*, Siaka Doumbia & Muhitdin Ahmetoglu  
Bursa Uludag University, Department of Physics, Bursa, Türkiye

Nickel oxide (NiO) thin films were fabricated by using reactive DC magnetron sputtering onto the soda lime glass substrates. NiO coated glass substrates were used for structural analyses. High purity Ni target was used as Ni source. The coating was carried out under 80% Ar-20% O<sub>2</sub> gas mixture at 10 mTorr total pressure with 470 V gun potential and 2 Å/s evaporation rate. After evaporation, these samples were annealed at 150 °C during 10, 20 and 30 min. The XRD measurements (Fig.1a) and the UV-VIS absorption spectra (Fig.1b) confine the NiO structure<sup>2</sup>.

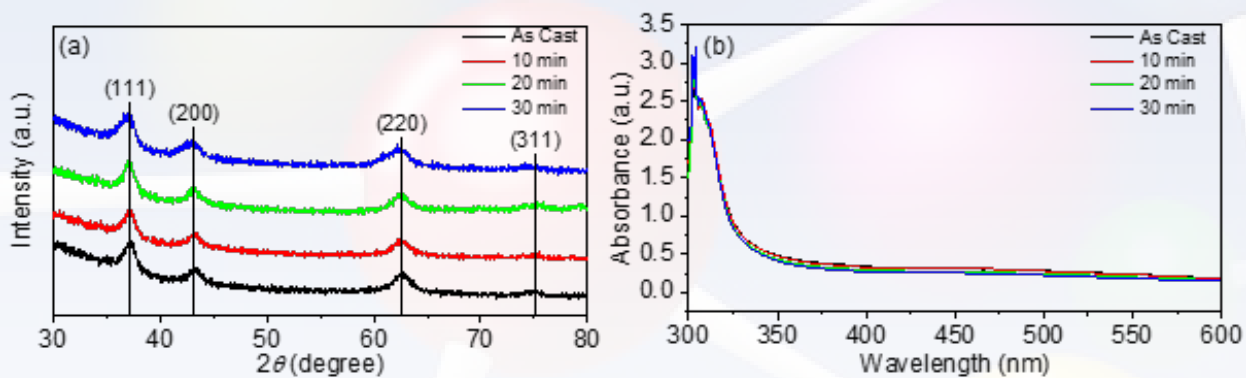


Figure 1. (a) UV-VIS spectra and (b) XRD graph of the NiO thin films on soda lime glass

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Nanoporous Si (NPSi) structures were synthesized by the MACE method<sup>1</sup> on one-side polished  $\eta$ -type Si (100) wafers. A 15-nm Cu film was thermally evaporated onto the whole surface of the polished side of the wafers. Cu source was 3N-grade copper pellets and deposition rate was 5 Å/s. The Cu-coated Si substrates were annealed at 150 °C in a tubular furnace under N<sub>2</sub> stream to prevent the oxidation for 15 min. The etching step was conducted in a solution of HF, H<sub>2</sub>O<sub>2</sub> and DI water at room temperature. The Cu film catalyzed the etching of the Si beneath it. The etching time was 30 min. The substrates were dipped into concentrated nitric acid solution to remove any Cu traces for 5 min after the etching. Then, NPSi substrates were loaded sputter system and coated by NiO, as mentioned above. Metal contacts were made by thermal evaporation using a mask, which have 1-mm diameter circular openings, onto NiO/*n*-type NPSi for the electrical characterization. These properties will also be discussed.

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### Biography:

M. Cuneyt Hacıismailoğlu received the Ph.D. degree in solid state physics from Bursa Uludağ University, Bursa, Türkiye, in 2011. He worked as honorary staff at the Department of Physics in University of Bristol, U.K., in 2012 and post-doctoral researcher with the Department of Chemistry, Middle East Technical University, Ankara, Türkiye in 2013 on white OLEDs. He is currently with the Department of Physics, Bursa Uludağ University as assistant professor. He is active in the fields of OLEDs, OPVs, photodiodes and solar cells.

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**Functional Ordered Nanoporous Materials Derived from Nanostructured Block Copolymers**

**Daniel Grande**

*Institut Charles Sadron, UPR 22 CNRS, 23 rue du Loess, 67034 Strasbourg, France*

Block copolymers have gained a tremendous interest from the scientific community in the last two decades. These macromolecular architectures indeed constitute ideal nanostructured precursors for the generation of nanoporous materials meant for various high added value applications. The parallel emergence of controlled polymerization techniques has notably enabled to finely control their molecular features to confer them with unique structural and physico-chemical properties, such as low dispersity values ( $\mathcal{D}$ ), well defined volume fractions, and controlled functionality. The nanostructuring and ordering of diblock copolymers, that can be achieved through various experimental techniques, including channel die processing, solvent vapor or thermal annealing, allows for the preparation of orientated microphase-separated copolymers whose morphology is dictated by three main factors, i.e. Flory-Huggins interaction parameter between constitutive blocks, volume fraction of the blocks, and polymerization degree. This lecture will provide an overview of the actual state of the art regarding the preparation of functional nanoporous materials from well-defined diblock copolymers. It will also highlight the major applications of such peculiar materials.

**Biography:**

Dr. Daniel Grande is a CNRS research director at Charles Sadron Institute (ICS) in Strasbourg where he moved in January 2024. Before his present position, he acted as the director of the ICMPE in Thiais for the period 2020-2023. He received his Ph.D. degree in polymer chemistry from the University of Bordeaux (France) and the University of Coahuila (Mexico) in 1998, and then he spent about two years at Emory University (Atlanta, USA) as a NIH post-doctoral fellow. his research interests include the development of functional polymer materials with a broad range of porosity scales, including nanoporous materials with controlled porosity and chemical functionality derived from polymer networks and nanostructured block copolymers, doubly porous materials with nano- and macro-porosity, as well as hybrid macroporous materials based on polymer fibers and inorganic nanoparticles.

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## Study of Flexible ZnSnO-channel-based Thin Film Transistors

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High-performance flexible ZnSnO-channel-high-entropy-dielectric-based thin-film transistors (TFTs) will be presented in this talk. Optimal high-entropy dielectric compositions with low equivalent oxide thicknesses were determined from a film library (wide composition space) deposited on indium tin oxide-coated glass substrates using high throughput processes. In addition to fundamental characterizations of compositions, microstructures, and constitutive elements, other advanced measurements indicated the formation of oxygen vacancies in the dielectric films and resulting high-entropy films. The film library was patterned to 450 metal-insulator-metal stacks, revealing their dielectric constants  $\approx 262-322$  and loss ( $\tan \delta$ )  $\approx 0.01-0.30$  at 1 kHz. The film library was further integrated to 63 TFTs and the promising ones exhibited remarkable parameters of an on/off current ratio of  $10^8$ , threshold voltage ( $V_T$ ) of 0.02 V, saturation field-effect mobility of  $184 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ , and subthreshold swing of  $0.062 \text{ V}\cdot\text{dec}^{-1}$ . The resulting TFTs also exhibited small and negligible changes in  $V_T$  and drain-source current, respectively, under various gate-bias stress conditions. Furthermore, rapid responses and impressive sensitivity and responsibility of the TFTs were obtained as UV detectors, and their excellent flexibility was implied by no substantial degradation in electrical and sensing characteristics when under various deformations. Our results indicate the great promise of high-entropy oxynitride films for next-generation flexible electronic devices.

### Biography:

Prof. Chang received his Ph.D. degree from the University of Maryland, College Park, MD USA. his research focuses on the exploration of functional nano-structured materials, including (1) low-k materials for 5G and 6G application, (2) piezophotocatalysis, (3) high- entropy high-k oxide films, (4) high-entropy piezoelectric films, (5) combinatorial (high throughput) physical and hydrothermal synthesis, and (6) electronic devices (MOS, MOSFET, TFT, and advanced TFT). He published more than 70 SCI papers with an h-index of 20. He delivered more than 20 invited talks at various international conferences, and is currently a managing guest editor for Thin Solid Films.

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## High-performance van der Waals antiferroelectric $\text{CuCrP}_2\text{S}_6$ -based memristors

Yinchang Ma and **Xixiang Zhang**

*Physical Science and Engineering, King Abdullah University of Science & Technology (KAUST), Saudi Arabia*

Layered thio- and seleno-phosphate ferroelectrics, such as  $\text{CuInP}_2\text{S}_6$ , are promising building blocks for next-generation nonvolatile memory devices. However, because of the low Curie point, the  $\text{CuInP}_2\text{S}_6$ -based memory devices suffer from poor thermal stability ( $<42^\circ\text{C}$ ). Here, exploiting the electric field-driven phase transition in the rarely studied antiferroelectric  $\text{CuCrP}_2\text{S}_6$  crystals, we develop a novel nonvolatile memristor showing a sizable resistive-switching ratio of  $\sim 1000$ , high switching endurance up to 20,000 cycles, low cycle-to-cycle variation, and robust thermal stability up to  $120^\circ\text{C}$ . The resistive switching is attributed to the ferroelectric polarization-modulated thermal emission accompanied with the Fowler–Nordheim tunneling across the interfaces. First-principles calculations reveal that the outstanding device performances are associated with the exceptional strong ferroelectric polarization in  $\text{CuCrP}_2\text{S}_6$  crystal. Furthermore, the typical biological synaptic learning rules, such as long-term potentiation/depression and spike amplitude/spike time-dependent plasticity, are also demonstrated. The results highlight the great potential applications of van der Waals antiferroelectrics in high-performance synaptic devices for neuromorphic computing.

### Biography:

Prof. Xi-Xiang Zhang earned his PhD from Universitat de Barcelona in 1992. He began as an assistant professor at Hong Kong University of Science and Technology, rising to full professor by July 2008. Moving to King Abdullah University of Science & Technology in 2008, he managed two core labs, later overseeing all in 2012. Since January 2014, he's been a full-time professor at KAUST. His diverse research encompasses magnetism, spintronics, nanomaterials, multiferroic and 2D materials. With 700+ co-authored papers and an H-index of 89, his work has garnered over 36,000 non-self-citations on Web of Science. He's also a APS fellow.

1. Yinchang Ma, et al. *Nature Communications* | (2023) 14:789



## Carbon materials for solar steam-generation

Masahiro Toyoda\* and Michio Inagaki

Faculty of Science and Technology, Oita University, 700 Dannoharu, Oita, 870-1124, Japan

Steam can be generated by solar illumination of nanoparticles suspended in water, which is called “solar steam-generation” and gets attention for the novel process for the production of drinkable water (water desalination). Recently, various carbon materials have been reported to be applicable for this process as solar energy absorbers (solar light receivers) with high conversion efficiency of light energy to thermal energy, mainly because of broad band solar absorption, capability for getting low bulk density (high porosity) to be self-floating on the water surface, etc., in addition to low costs for preparation. here, we reviewed SSG performances by focusing on carbon materials, by classifying in the porous carbons, including carbon foams and activated carbons, graphite-based carbons, including reduced graphite oxides and graphene oxide, fibrous carbons, including carbon fibers, carbon nanofibers, carbon nanotubes and their clothes and webs, and biomass-derived carbons. The applicability of biomass-derived carbons prepared through simple carbonization processes to SSG process can reinforce the conformability to the coming “carbon neutral society”. Recent results on co- generation of electric power with water desalination are also reviewed.

In the coming “carbon neutral society”, the production of carbon materials has to be performed from sustainable precursors, i.e., mainly biomasses, not from polymers synthesized from various fossils, coals, oils and natural gases, which had been used so long period since the first industrial revolution.

All of us are asked to change revolutionary our science and technology for carbon materials to conform to the “carbon neutral society”. The study on biomass-derived carbons for SSG technique may give us the first chance (first challenge) to establish a new science and technology of carbon materials for the “carbon neutral society”

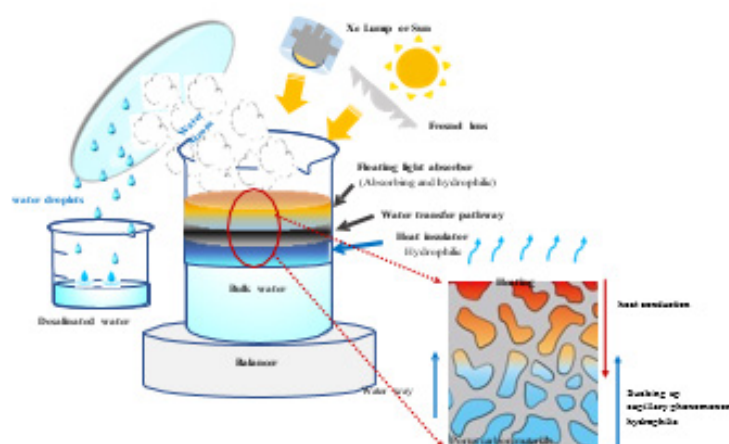


Fig. Schematic illustration of solar steam-generation [1].

[1] M. Toyoda and M. Inagaki, Carbon materials for solar steam-generation, *Carbon*, 214, 118373(2023).

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**PROMOTING SUSTAINABILITY THROUGH NEW ADVANCES IN THE PRODUCTION OF LITHIUM-ION BATTERIES AS PART OF THE BATWOMAN PROJECT**

**Bernd Eschelmüller<sup>1</sup>, Katja Fröhlich<sup>1</sup>**

<sup>1</sup> *Battery Technologies, AIT Austrian Institute of Technology GmbH, Giefinggasse 2, Vienna, Austria*

The main objective of BatWoMan is to develop novel, cost-effective and environmentally friendly methods for lithium-ion battery cell production. This presentation gives an overview of the innovative strategies and technologies being undertaken to achieve this goal. It highlights the potential to advance the European Union's ambitious goal of realizing the production of carbon-neutral energy storage systems, while promoting economic feasibility and environmental protection.

BatWoMan focuses on three key technological efforts. Firstly, it concentrates on the development of energy-efficient processes for electrode production with elimination of volatile organic components and processing highly concentrated slurries of up to 70% and 80% by weight for anode and cathode respectively.

Secondly, the project will implement breakthrough concepts to reduce dry room needs, significantly lowering the cost of cell production and minimizing the carbon footprint of the entire battery manufacturing process. Given that the operation of the dry room is a major cost component in the battery production value chain, these innovations hold immense potential for reducing costs and environmental impact. In addition, a battery data space will be established to ensure traceability and condition determination of the battery cells produced and to increase transparency for customers and second-life users.

Finally, BatWoMan establishes cost-effective and energy-efficient cell conditioning methods that include wetting, formation, and ageing processes.

Three-dimensional electrode designs are being developed to improve the cell conditioning steps and ensure optimal performance and extended lifetime of lithium-ion cells. These advances are expected to improve the overall sustainability and economic viability of future environmentally friendly batteries at the cell level.

Through these efforts, BatWoMan will significantly reduce cell production costs by 63.5% and reduce energy consumption in cell production by 52.6%, positioning Europe as a leader in sustainable battery production. This project has received funding from the European Union's Horizon research and innovation programme under Grant Agreement no. 101069705

**Biography:**

The author, Bernd Eschelmüller, works as a Research Engineer at the AIT Austrian Institute of Technology GmbH, Vienna, Austria, in the group 'Battery Technologies' on pioneering research projects in the field of battery cell production. In addition, the author has in-depth knowledge of the planning, execution, and management of projects in the fields of research and pilot plant engineering. With the special experience he has gained in the areas of process development for electrode production and battery cell construction, the researcher is currently working on the BatWoMan project to develop sustainable and environmentally friendly processes for the cell production of tomorrow.

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### **Hot Rolling of Ta-B and Ta-Al-B(B4C) Reactive Blends.**

**Akaki B. Peikrishvili\***, Zaqaria Melashvili, Teimuraz Namicheishvili, Zurab Aslamazishvili and Neli Goniashvili,  
*Ferdinand Tavadze Institute of Metallurgy and Materials Science, Tbilisi, Republic of Georgia*

The Ta-B and Ta-Al-B(B4C) reactive blends were rolled and formed into sheets by combining self-propagating high temperature synthesis (SHS) and hot electrical rolling processes.

The aim of the investigation was to synthesize and to fabricate in one stage near to theoretical density composites of TaB<sub>x</sub> and Ta<sub>x</sub>Al<sub>y</sub>-TaB<sub>x</sub> (B4C) having perfect structure and high value of strength properties.

The preliminary calculation showed that in order to create a sufficient thermal effect for the SHS reaction and to provide rolling process in a stable manner it is necessary that during the rolling the exothermic reaction of the SHS process provide a temperature range in the sample of 1300- 2300K. At the beginning of rolling process an electric current is passed in the charge through the deformation zone and due to the release of “Joule” heat the SHS process is initiated. The synthesized porous sample with a predetermined delay is continuously fed towards to deformation zone for further consolidation-densification.

The investigation showed that the combination of electrical rolling method with SHS process was beneficial to the consolidation & syntheses of the Ta<sub>x</sub>Al<sub>y</sub>-TaB<sub>x</sub> composites, resulting in near theoretical densities, high hardness values, and the formation of different intermetallic compounds of Ta<sub>x</sub>Al<sub>y</sub>. The structure and hardness of the sheets obtained, depended on the loading conditions and the phase content of starting blends.

It was found that in order to obtain high density sheets by SHS-Electric rolling combined method, it is necessary to comply with the condition and to maintain a constant distance between the cross section of the synthesis front and deformation zone. It is established that excess consolidated and synthesized mass shifts towards the direction of least resistance, the more porous rear part of the workpieces. As a result, the length of the rolled product from the input section of the deformation zone increases that violates the condition of a constant distance between the combustion front and the deformation zone. In order to maintain established rolling condition, it is necessary to increase the feeding speed to such a value that the synthesized mass enters to the deformation zone in a homogeneous viscoplastic state.

The processing temperature at the beginning of rolling were changed from 1000 up to 1300 K The intensity of compression was below the 60MPa.

**This work was supported by Shota Rustaveli National Science Foundation of Georgia – SRNSFG (Grant number STEM-22-1113).**

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**Biography:**

Akaki Peikrishvili (PhD, Dipl. Engineer) is a head of laboratory of Tavadze Institute of Metallurgy and Materials Science. 2001-2018 the coordinator and head of the Office of STCU ([www.stcu.int](http://www.stcu.int)) in Georgia Dr. Peikrishvili's has led and participated in more than 200 international scientific projects and award contracts, including projects with BNL and LLNL of DOE USA and US Army Research Laboratory. He is a frequent speaker at international conferences and symposiums. Dr. Peikrishvili is Certified Expert on explosive engineering. He has published more than 120 scientific articles in Georgian and International journals/proceedings in the field of materials science and nanotechnology.

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## High-entropy alloys with excellent mechanical properties and irradiation resistance

**Haiming Wen**

*Missouri University of Science and Technology, Rolla, Missouri, USA*

Conventional alloy design based on single-principal element systems limits the space and flexibility to explore alloy chemistries and optimize microstructures. The concept of multi-principal element alloys, or high-entropy alloys (HEAs), has revolutionized traditional alloy design strategies, creating tremendous opportunities to explore new alloys in the vast compositional space. Some HEAs have been reported to possess significantly improved mechanical properties over conventional alloys, such as high strength-weight ratio, fracture resistance, high-temperature strength and structural stability. However, the specific properties depend on the specific composition, processing and microstructure, and the composition-process-structure-property relationships need to be well understood. Furthermore, HEAs have been proposed to possess significantly enhanced irradiation tolerance. Nevertheless, irradiation studies of HEAs (especially precipitation-strengthened ones) are limited and mechanisms underlying irradiation behavior remain poorly understood. Most HEAs developed so far contain Co, which are not suitable for nuclear applications. In this study, solid-solution or precipitation-strengthened HEAs with different compositions (including Co-free ones) and microstructures were processed by conventional manufacturing (casting followed by rolling and heat treatment) or advanced manufacturing techniques (including powder metallurgy route involving rapid sintering, and severe plastic deformation). The microstructure of the fabricated HEAs were carefully studied utilizing advanced microstructural characterization techniques. Mechanical properties and irradiation behavior were investigated. Results indicated that excellent mechanical properties including high-temperature strength were achieved, as well as enhanced irradiation tolerance. This study provides insights to optimize the design and processing of HEAs to achieve superior mechanical and physical properties.

### Biography:

Dr. Haiming Wen is an Associate Professor in Department of Materials Science and Engineering at Missouri University of Science and Technology. He obtained his PhD from University of California, Davis. Dr. Wen has extensive experience in research and development of advanced materials, especially those for extreme environment applications. Dr. Wen has authored or coauthored >85 peer-reviewed journal publications, with citations >4,300 and an h-index of 27. He serves on the Editorial Board of the journal Materials Science and Engineering A. He was named CEC Dean's Scholar, and received an Outstanding Teaching Award and a Faculty Research Award from Missouri S&T.

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**Modulation of electrical, acoustic and optical properties of phthalocyanines by gas adsorption: interest for gas sensors development.**

**J. Brunet**<sup>\*1</sup>, H. Bruhier<sup>2</sup>, A. Ndiaye<sup>1</sup>, S. Rajab-Pacha<sup>1</sup>, C. Varenne<sup>1</sup>, A. Pauly<sup>1</sup>, Y. Jourlin<sup>2</sup>

<sup>1</sup> *Université Clermont Auvergne, Clermont Auvergne INP, CNRS, Institut Pascal, F-63000 Clermont-Ferrand, France*

<sup>2</sup> *Université Jean Monnet Saint-Etienne, CNRS, Institut d'Optique Graduate School, Laboratoire Hubert Curien UMR 5516, F-42023, SAINT-ETIENNE, France*

Phthalocyanines constitute an extended family of molecular semi-conductors that possess specific optical, electrical and adsorption properties due to their high aromaticity and the extended delocalization of  $\pi$ -electrons. The adsorption of various gases can lead to the modulation of these properties involving different interactions between gases and materials: redox reaction,  $\pi$ -stacking, repulsion forces. Thus, the electronic conductivity, the mass and the optical index of phthalocyanine layers can be significantly modified by gas even for very low concentrations. Such sensing materials appear as highly relevant for the development of chemical micro-sensors exhibiting high sensitivity, low limit of detection and high resolution. The selectivity can be performed by the implementation of appropriate transducers: conductimetric, acoustic or optical.

This lecture is focused on the gas/phthalocyanines interaction mechanisms and their effects on material properties. Strategies for the elaboration of gas sensors dedicated to target gases are described. The key role of transducer on the discrimination of the target gas is highlighted. Illustrated by relevant results, it is manifest that phthalocyanines layered on conductimetric transducers give highly selective sensor responses to nitrogen dioxide  $\text{NO}_2$  while selective responses towards aromatic hydrocarbons (BTEX) are obtained with acoustic transducers. In contrast, phthalocyanines associated to surface plasmon resonance transducer deliver higher responses to ammonia  $\text{NH}_3$ . Beyond selectivity, metrological performances of all micro-sensors will be assessed and discussed.

**Biography:**

Jérôme BRUNET has obtained his Ph.D. degree in material science and components for electronic from Université Blaise Pascal, France, in 2003. Since 2004, he is working as an Associate Professor in the Chemical Microsensors and Sensor-Systems division at the Institut Pascal laboratory (Clermont Auvergne University). his research is focused on the development of acoustic, conductimetric and plasmonic microsensors as well as sensor-systems implementing nanocarbons, phthalocyanines and hybrid materials as sensing materials for the monitoring of gas at very low concentrations. Since 2021, he's the team leader of his Chemical Microsensors and Sensor-Systems group.

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## Essential oil-loaded coaxial wet-spun fibers for wound healing applications

Catarina S. Miranda<sup>1,\*</sup>, Elina Marinho<sup>1</sup>, Catarina Leal Seabra<sup>2</sup>, Camille Evenou<sup>3</sup>, Jérôme Lamartine<sup>3</sup>, Berengere Fromy<sup>3</sup>, Susana P.G. Costa<sup>4</sup>, Natália C. Homem<sup>5</sup> and Helena P. Felgueiras<sup>1</sup>

<sup>1</sup> Centre for Textile Science and Technology (2C2T), University of Minho, Campus of Azurém, 4800-058 Guimarães, Portugal

<sup>2</sup>Associate Laboratory for Green Chemistry (LAQV), Network of Chemistry and Technology (REQUIMTE), Department of Chemical Sciences, Faculty of Pharmacy, University of Porto, 4050-313 Porto, Portugal

<sup>3</sup>Équipe Intégrité fonctionnelle du tissu cutané (SKIN). Laboratoire de biologie tissulaire et d'ingénierie thérapeutique (LBTI), CNRS UMR5305, Université Lyon I, 7 passage du Vercors, 69367 Lyon Cedex 07, France

<sup>4</sup>Centre of Chemistry (CQ), University of Minho, Campus of Gualtar, 4710-057 Braga, Portugal

<sup>5</sup>Simoldes Plastics S.A., Rua Comendador António da Silva Rodrigues, 165, 3720-193, Oliveira de Azeméis, Portugal

Chronic wounds (CWs) are frequently associated with bacterial infections. The development of antibiotic-resistant microorganisms makes it crucial to think of alternative solutions. Considering these issues, a drug delivery system made of coaxial wet-spun fibers loaded with essential oils (EOs) was proposed. Coaxial structures were produced using the wet-spinning technique, in which 10% w/v polycaprolactone (PCL, a synthetic polymer with excellent mechanical properties and elastic behavior) was used to produce the core and loaded with three EOs, Clove Oil (CO), Cinnamon Leaf Oil (CLO) and Tea Tree Oil (TTO) at 2×Minimum Bactericidal Concentration (MBC). The shell was made of a blend of 10% w/v cellulose acetate (CA, a natural polymer which has been reported to offer good structural integrity) and 10% w/v polyethylene glycol (PEG, a synthetic polymer often used as a plasticizer), mixed at a ratio of 90/10 v/v, respectively, so pores could be opened in the outer layer, allowing for a sustained release of the EOs loaded at the fibers' core overtime. The formation of coaxial structures was confirmed by brightfield microscopy. Coaxial fibers

exhibited high maximum elongations at break ( $\approx 350\%$ ). EO-loaded fibers were effective against *Staphylococcus aureus*, *Staphylococcus epidermidis*, *Escherichia coli* and *Pseudomonas aeruginosa*, the most common bacteria present in CWs. In addition, all three EOs showed a prolonged and sustained release profile and all the engineered fibers did not cause any cytotoxic effects after being in contact with human keratinocytes (HaCaT) and mouse embryonic fibroblasts (NIH 3T3). Results confirmed the potential and safety of the engineered coaxial wet-spun fibers for potential wound healing applications.

### Biography:

Catarina S. Miranda completed in 2020 an integrated master degree in Biomedical Engineering in the University of Minho, Portugal. In the same year she was granted with a PhD scholarship of 4 years in the same university (2020.08547.BD). Since then, she dedicated her research into producing medical textiles for wound healing applications. Currently, she is in the final year of her PhD and main author of 2 review articles, 1 research article and 1 conference paper, along with several conference posters and oral presentations. her main goal is to improve the population's health and quality of lives with her research.

*Keynote Talks*  
**DAY-2**



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**Advanced Handheld Spectroscopic Eye-Safe Technology for Point-Of-Care Detection of Traumatic Brain Injury**

**Pola Goldberg Oppenheimer**

*School of Chemical Engineering, Institute of Healthcare technologies, University of Birmingham, Edgabston, Birmingham, B15 2TT, United Kingdom*

Traumatic brain injury (TBI), a major cause of morbidity and mortality worldwide, is hard to diagnose at the point of care with patients often exhibiting no clinical symptoms. TBI injuries evolve immediately after the initial trauma, yet many individuals display very few clinical symptoms at the early stages, which, however subsequently, develop long-term, persistent, neurodegenerative deficits. As the brain tissue lacks regenerative capacity, early diagnosis is crucial for improving outcomes. Life critical decisions, which influence patients' prognoses and the efficacy of treatment, must be made within the first hour after trauma. There is an urgent need for rapid point-of-care diagnostics to enable timely intervention. We have developed a technology for rapid acquisition of molecular fingerprints of TBI biochemistry to safely measure proxies for cerebral injury through the eye, providing a path toward noninvasive point-of-care neurological diagnostics using simultaneous Raman spectroscopy and fundus imaging of the neuroretina. Detection of endogenous neuromarkers in porcine eyes' posterior revealed enhancement of high-wave number bands, clearly distinguishing TBI and healthy cohorts, classified via our advanced artificial neural network algorithm for automated data interpretation as a decision support tool of the self-optimizing Kohonen index network (SKiNET). SKiNET as a framework for an advanced multivariate analysis, simultaneously provides (i) dimensionality reduction, (ii) feature extraction, and (iii) multiclass classification to identify the underlying chemical differences between classes, providing accurate classification for simultaneously rich-information and high classification specificity, even for low laser powers and short acquisition times, representative of the real-world point-of-care conditions. Clinically, translating into reduced specialist support, this markedly improves the speed of diagnosis. Designed as a hand-held cost-effective technology, it can allow clinicians to rapidly assess TBI at the point of care and identify long-term changes in brain biochemistry in acute or chronic neurological diseases.

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**Biography:**

Pola Goldberg Oppenheimer is a Professor in Micro-Engineering and Bio-Nanotechnology at the School of Chemical Engineering and the Healthcare Technologies Institute (HTI). Professor Oppenheimer leads an interdisciplinary research group at the University of Birmingham, closely working with the clinical teams at the Queen Elizabeth Hospital (QEHB) and Birmingham Enterprise, the University's technology transfer specialists. her group's research programme is targeted at exploring the frontiers of micro to nanomaterials engineering while bridging the gap between nano-to-macroscopic-level understanding and implementations of novel hybrid and nanocomposite materials and submicron structures for miniaturised functional devices for advanced healthcare applications. Professor Oppenheimer is developing cutting-edge Engineering solutions to tackle major medical problems. Professor Oppenheimer's research interests lie in nano and submicron structure formation (Advanced Nano-Materials, Structures and Applications Group) at surfaces and in thin films, including pioneering the potential use of hierarchical electrohydrodynamically generated functional structures to develop novel polymer-based nano-detection devices. She brings detailed expertise in creating and aligning a wide range of nanostructures in polymers, carbon nanotube-based nanocomposites, crystalline materials and a synergistic interest in biometrics, including the use of polymers with 10mm morphologies as templates to create inorganic functional devices.

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**Protein interaction analysis by surface plasmon resonance and application**

**Dennis G. Drescher\*** and Marian J. Drescher

*Wayne State University, Detroit, Michigan 48201, U.S.A.*

Surface plasmon resonance (SPR) is an optical technique utilized for detecting molecular interactions, such as the binding of one protein to another. Binding of a mobile protein (analyte) to a second protein immobilized on a thin metal film (ligand) changes the refractive index at the film surface. The angle of extinction of 760 nm light reflected after polarized light impinges upon the film is altered and monitored as a change in detector position, for a dip in reflected intensity due to resonant conversion of photons to plasmons. Because the method strictly detects mass, there is no need to label interacting components. Binding affinities can be obtained either from the ratio of rate constants or from measurement of the steady state level of binding as a function of binding-partner concentration. The high sensitivity of SPR (1 nmol for proteins) makes the methodology ideal for studies of the inner ear, where only small amounts of pure protein are available. For example, a major synaptic complex protein, syntaxin, has been shown to bind, by SPR, to the N-type voltage-gated calcium channel of the sensory hair cells of the vestibular saccular macula. This binding is calcium-dependent and completely abolished in the presence of calcium chelators. These results suggest that the influx of calcium during hair-cell stimulation is linked to interaction of the calcium channel with the synaptic complex, promoting release of transmitter, for perception of balance and hearing. Further, a cyclic nucleotide-gated ion channel, CNGA3, was shown by SPR to interact with myosin VIIa in a calcium-dependent manner. Since CNGA3 and myosin VIIa are proteins both thought to be involved in hair-cell mechanotransduction, their calcium-dependent interaction is consistent with functioning in the conversion of mechanical to electrical signal. Thus, SPR serves as a useful tool to examine molecular mechanisms integral to biological function.

**Biography:**

Dennis G. Drescher is Professor and Director of Molecular Research in the Department of Otolaryngology and Professor in the Department of Biochemistry, Wayne State University School of Medicine, Detroit, Michigan, USA. He obtained his Ph.D., M.M. and B.S. degrees from the University of Wisconsin, Madison and pursued postgraduate studies in biochemistry at Harvard University, Cambridge, Massachusetts. He has served as Senior Staff Fellow at the NIH, Bethesda, Maryland and Research Associate at Washington University, St. Louis, Missouri. his interests include interactions of synaptic-complex and mechanotransduction proteins of the inner ear as analyzed by surface plasmon resonance.

*Scientific Session*

**DAY-2**

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**Flame retardant chicken feather/polypropylene composites – a novel approach towards efficacy improvement with improved feasibility**

Avishek Mishra and Debes Bhattacharyya

*Centre for Advanced Materials Manufacturing and Design, Department of Mechanical Engineering, The University of Auckland, Private Bag, Auckland 92019, New Zealand*

This research explores the integration of waste materials into product development strategies, focusing on the use of chicken feather fibres as reinforcements in polypropylene (PP) composites to improve flammability performance [1,2]. The incorporation of ammonium polyphosphate (APP) as a flame retardant additive is traditionally employed but presents challenges in maintaining the mechanical properties and overall economic feasibility. Our approach produces flame retardant chicken feathers (FRCF) while minimizing the environmental impact and processing costs.

The presence of 44 wt.% FRCF led to about 80% reduction in peak heat release rate (PHRR) compared to that of polypropylene alone. FRCF in the composite also partially overcame the detrimental effects of APP on the interfacial adhesion between fibre and polymer. Cone calorimeter tests have demonstrated a reduction of ~21% in the fire growth rate and delayed PHRR, indicating improved fire performance in the combined presence of FRCF and a significantly reduced amount of APP. Additionally, the reduction in tensile strength of the composite was arrested, indicating an improved interfacial bonding.

Evaluation of the green chemistry aspects has involved the comparison of physical mixing and chemical incorporation of melamine phosphate onto chicken feathers. The cost of production of 1 kg of FRCF-reinforced polypropylene composites has been calculated to be ~33% less than its commercial counterpart. While both methods of producing FRCF have comparable environmental factor (Ef), the chemical process exhibits almost 50% lower wastewater intensity and improved atom utilization (~11%), highlighting its efficiency and environmental benefits [3,4].

This study underscores the potential of utilizing waste materials, such as chicken feathers, in the production of sustainable composites. By addressing both environmental concerns and performance requirements, the approach aligns with the principles of green chemistry and offers promising avenues for enhancing the sustainability of engineering polymers.

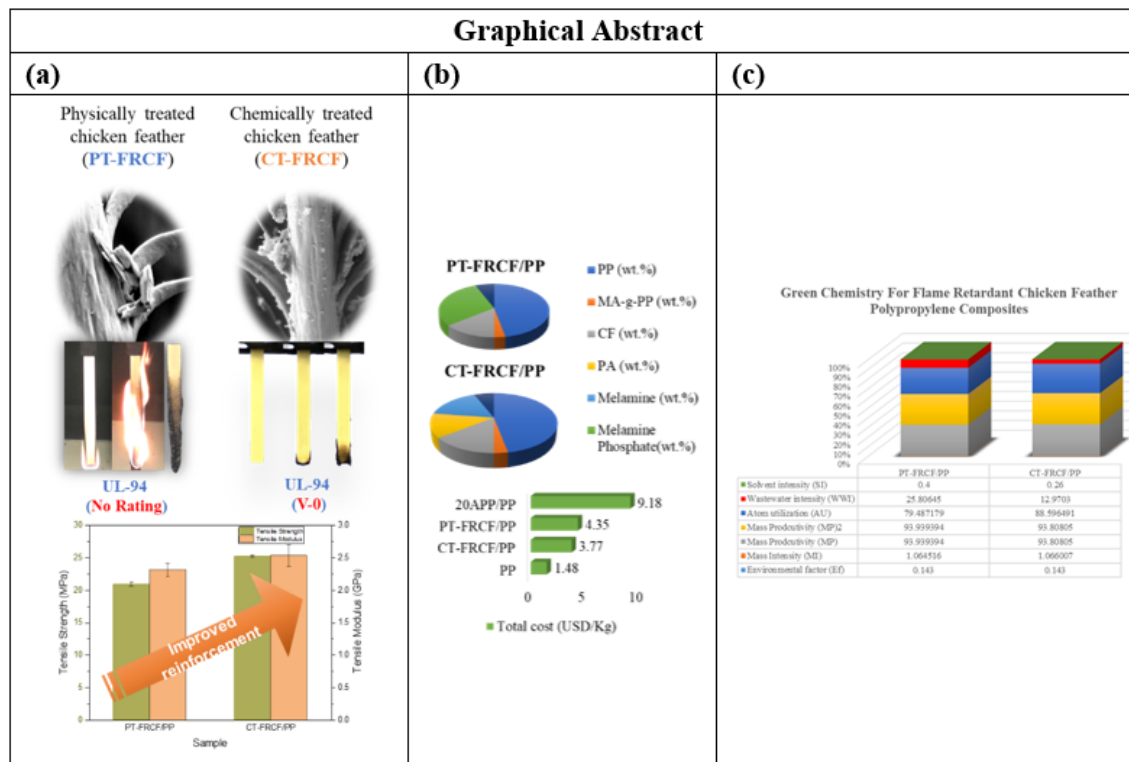


Figure 1. (a) UL-94 test and mechanical performance for PT-FRCF and CT-FRCF composites; (PT-FRCF: Physically treated Flame retardant chicken feathers; CT-FRCF: Chemically treated Flame retardant chicken feathers); (b) The pie chart represents individual constituents wt.%, and the bar chart represents the cost of production for 1kg of each composites in USD (c) The physical and chemical treatment processes greenness values

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**Biography:**

Dr. Debes Bhattacharyya is currently a Distinguished Professor Emeritus in the Department of Mechanical Engineering, University of Auckland, New Zealand. He has served as the Head of Mechanical (& Mechatronics) Engineering Department and as the founding Director of Centre for Advanced Composite Materials. In 2016, he was felicitated as the Dr APJ Abdul Kalam Professor by SRM University in Chennai, India. For many years he was an Adjunct Professor at Washington State University, Pullman, USA. his research involves the mechanics and manufacturing of composite materials yielding >550 publications including several edited/ authored books and some chapters. He is a Fellow of the Royal Society, NZ and a Distinguished Fellow of EngNZ. He has an honorary 'Doctor of Engineering' (*honoris causa*), awarded by the USQ, Australia, and received the Supreme Technical Award from EngNZ. He has supervised more than 110 postgraduate students including 68 doctoral candidates.

# 7<sup>th</sup> International Conference on **Materials Science & Nanotechnology** July 15-16,2024 at Vienna, Austria (Hybrid Event)



## High-Performance Air-Stable Solar Selective Absorber for CSP Applications up to 450 °C

**Meryem Farchado**<sup>1,2\*</sup>, Naia Barandica<sup>1,2</sup>, Gema San Vicente<sup>1</sup>, Nuria Germán<sup>1</sup>, Aránzazu Fernández-García<sup>3</sup> and Ángel Morales<sup>1</sup>

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The current energy crisis, with an increase of about 54 % in total carbon oxide emissions in recent years, requires an urgent decarbonisation of the economy. Therefore, it is imperative to develop alternative energy sources. Among the current renewable energy sources, solar energy is considered a good candidate to replace fossil fuel sources. Specifically, solar thermal conversion technology that allows the solar energy to be harnessed in an easy and immediate way has attracted increasing interest during the last decades. Its excellent temperature adaptability and the concern to improve the efficiency of Concentrated Solar Thermal (CST) systems convert the development of Spectrally Selective Absorber Coatings (SSACs) in an active research field. The ability of SSACs to ensure a high absorptance ( $\alpha_s$ ) of solar irradiation in the solar wavelength range (0.3-2.5  $\mu\text{m}$ ) and low thermal emittance ( $\epsilon_T$ ) in the mid/far-infrared wavelength ranges ( $>2.5 \mu\text{m}$ ) makes these materials potential candidates for guaranteeing high thermal efficiency in CST systems. Up to now, there has been a lack of commercial competitors, achieving the SSAC most commonly used for the parabolic trough collector (PTC) receiver tube the optical properties in vacuum of  $\alpha/\epsilon_{400^\circ\text{C}} = 0.960/0.095$  [1]. However, this material undergoes an important degradation once the tube is exposed to air as a consequence of vacuum loss. Therefore, it is undisputable the importance of designing new high temperature air stable selective absorbers to increase current efficiency, simplify manufacturability and reduce costs. Within the I+D+i Project INTECSOL (PID2021-126664OB-I00), CIEMAT-PSA developed by dip-coating methodology a novel multilayered configuration of SSA stable in air for temperature applications up to 450 °C. This material achieved competing optical properties ( $\alpha_s > 0.95/\epsilon_{400^\circ\text{C}} = 0.08$ ) and exhibited excellent stability in air at 400 °C indicating its capability of maintaining its selective properties even if the vacuum is breached.

### Biography:

Bachelor in Chemistry Sciences and Master in Chemical Science and Technology from Universidad Complutense de Madrid. She contributed to different research topics: preparation and characterisation of solar selective absorbers for low-temperature applications (CIEMAT-PSA, Spain) and design of a thermal energy storage system using an Al redox-cycle to integrate into Swiss houses (SPF Institute for Solar Technology, Switzerland). In 2020 she joined as a pre-doctoral candidate at the Universidad Autónoma de Madrid the Unit of Materials for Concentrating Solar Thermal Technologies in CIEMAT-PSA. During the Ph.D., she acquired special experience in the design, preparation by sol-gel and dip-coating techniques, and characterisation of materials for solar thermal applications.

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## **Active Control of Springback Effect in Deep Drawing Processes: Theory and Experiment**

**Mostafa Mehrabi**

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Deep drawing is a sheet metal forming process in which a metal blank is radially drawn into a forming die by the mechanical action of the punch. Dimensional tolerances and their variations are important aspects of quality control issues in this forming operation. During this process, the workpiece goes through some work hardening and, therefore, some residual energy is released in the final stage, which results in further deformation of the part (so-called “springback”). There are several parameters that affect springback, and they can generally be classified as design parameters, material properties, and process variables. This research is mainly focused on process-related variables and their impact on dimensional variations and the final quality of the part. A parametric study is carried out by using DOE as a tool. This provides one with a better understanding of the severity of the impact of changes in these parameters and their effects on springback. An experimental setup is designed and developed that is used for this purpose. In this research, the impacts of various process parameters such as lubrication, punch speed, punch and die nose radius, blank holding force and material properties are studied, and the results are reported. The experimental results are used in the DOE to systematically analyze the effects of the process parameters and their relative contribution in the springback phenomenon. A simulation study of the process is carried out and the experimental results obtained from this setup are also used to analyze and validate the accuracy of simulation results in predicting performance when a parameter is changed. A comparison is made between the results obtained from the experimental setup and those obtained from simulation, and the results are reported. Study of control strategies to reduce springback is another contribution of this research work. In this regard, a control strategy is developed that is suitable for real-time control applications to reduce springback effects in deep drawing. Performance of this control strategy is studied in simulation of the process, and the results are presented.

## Hall-Petch Equation: a possible modification for submicron-grained metals

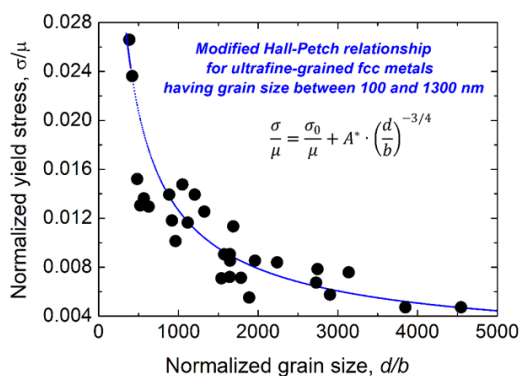
Nguyen Q. Chinh

Department of Materials Physics, Eötvös Loránd University, ELTE 1117 Budapest Pázmány Péter sétány 1/A, Hungary

The well-known Hall-Petch equation is used successfully to describe the relationship between the average grain size ( $d$ ) and yield strength of a polycrystalline material above 1  $\mu\text{m}$  average grain size for 70 years, showing a well established linearity between the yield strength and reciprocal of the square root of grain size. Thanks to the advances in grain refining techniques, numerous studies have been carried out on materials with grain structures at the sub-micron and nanocrystalline scale. These studies have shown that at such small grain sizes the Hall-Petch formula cannot be maintained in its original state. In this work, an appropriate modification of the Hall-Petch relationship is suggested to provide a uniform description of the grain size strengthening of submicron-structured face-centered cubic (f.c.c.) metals and solid solution alloys.

**Keywords:** f.c.c. metals, grain size strengthening, Hall-Petch relationship, strength of polycrystals, submicron-grained structures.

**Reference:** Nguyen Q. Chinh et al, MSEA 862 (2023) 144419.



**Figure 1:** Presentation of the normalized yield stress-normalized grain size relationship, proposing a modification of the Hall-Petch relationship for ultrafine-grained fcc metals and solid solutions.

### Biography:

"Prof. Nguyen Quang Chinh, Doctor of Science (DSc) from the Hungarian Academy of Sciences (HAS), graduated in Physics from Eötvös Loránd University (ELTE) in 1985. Since then, he has been working in various fields of materials science. His recent main research topics are: i) Plastic behavior and strengthening mechanisms of metals and alloys, ii) Microstructural and mechanical characteristics of ultrafine-grained and nanocrystalline materials, iii) Development of the depth sensing indentation method. He participated in many international collaborations. Currently, he is the leader of the Hungarian group in a joint project with Russian researchers entitled "Study of the physical nature and development of ultra-low-temperature superplasticity in ultrafine-grained Al alloys for innovative applications".

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**Fabrication of 3D printed devices coated with thiol-grafted iron-based metal organic framework for heavy metal removal**

Daniel Roberto Sáenz García<sup>1,2\*</sup>, Andreu Figuerola<sup>2</sup>, Gemma Turnes Palomino<sup>2</sup>, Luz O. Leal<sup>1</sup>, and Carlos Palomino Cabello<sup>2</sup>

<sup>1</sup> Environment and Energy Department, Advanced Materials Research Center, (CIMAV) S.C., Miguel de Cervantes 120, Chihuahua, Chih. 31136, Mexico

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Ensuring safe drinking water is an indispensable task for the survival of humans and wildlife. Heavy metals are a high importance class of pollutants, due to their high toxicity, even at trace amounts, persistence in the environment, mobility, bioaccumulation, and the impossibility of degradation<sup>1</sup>. Metal organic frameworks (MOFs) have emerged as promising materials for adsorbing pollutants, owing to their properties such as high surface area, stability against chemical and thermal influences, and tuneability. However, the synthesis of MOFs results in a microcrystalline powder limiting its practical applicability<sup>2,3</sup>.

In this work, we propose the synthesis of the MIL-100(Fe) MOF and its post-synthesis modification with thiol groups using a simple grafting procedure. The addition of thiol groups enhances the affinity, thereby increasing the extraction of heavy metals ions. MIL-100(Fe)-SH was mixed with a solution of PVDF/DMF to create an ink, subsequently applied as a coating onto 3D printed supports. The 3D printed device was designed to accommodate a magnetic stirrer, serving as stirrer and sorbent. The 3D printed coated device effectively extracted Hg(II), As(V), and Pb(II) from various water samples using an optimized procedure (pH and extraction time). Its recyclability remained high, nearing 100%, even after 5 cycles.

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#### Acknowledgements

Daniel Roberto Sáenz García expresses gratitude to the National Council of Humanities, Science and Technology in Mexico and Santander-UIB for the scholarship.

#### Biography:

Daniel Roberto Saenz Garcia holds a bachelor's degree in chemistry from the Autonomous University of Chihuahua. He obtained dual master's degrees from the Advanced Materials Research Center (CIMAV, Mexico) and the Balearic Island University (UIB, Spain). Currently, he is pursuing a dual Ph.D. at CIMAV/UIB under the guidance of Carlos Palomino Cabello and Luz O. Leal Quezada. his research concentrates on the developing of low-cost automatized systems, employing metal-organic frameworks and open-source platforms for environmental pollutant monitoring.

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## **Spin-polarized electronic states of high- $T_c$ cuprate superconductors**

**Hideaki Iwasawa**

*National Institutes for Quantum Science and Technology (QST)*

In high-temperature (high- $T_c$ ) cuprate superconductors, electron correlations are generally considered the dominant interaction. However, the spin-orbit interaction has often been overlooked or treated as a minor perturbation, leading to insignificant effects on the electronic ground state of these materials. Recently, a report has suggested the importance of spin-orbit interaction based on experimental observations of spin-polarized electronic states [1]. Nevertheless, the complexity of the spin texture reported has left the origin of spin polarization in high- $T_c$  cuprates unclear. In this work, we will present the spin- and angle-resolved photoemission spectroscopy (spin-resolved ARPES) study on single and bilayer Bi-based high- $T_c$  cuprates [2]. We consistently found very weak spin polarization only along the nodal direction, with no indication of spin-splitting of the band. Our findings thus call for a revision of the simple application of the spin-orbit interaction, which has been treated within the standard framework of the Rashba interaction in high- $T_c$  cuprates.

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### **Biography:**

Hideaki Iwasawa is a project leader of the Quantum Matter Measurement Informatics Project at National Institutes for Quantum Science and Technology (QST) in Japan. He received his Ph.D. in Physics from Tokyo University of Science, focusing on the electronic structures of strongly correlated electron systems, such as layered perovskite superconductors using angle-resolved photoemission spectroscopy (ARPES). He has extensive experience in developing and utilizing ARPES systems at synchrotron facilities, the Hiroshima Synchrotron Radiation Center (HiSOR), and Diamond Light Source. He is currently working on developing a novel ARPES beamline with superior spatial resolutions at a new synchrotron facility, NanoTerasu, in Tohoku, Japan. His recent research has focused on microscopic electronic structures of quantum materials by combining spatially-resolved ARPES and measurement informatics.

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## A nano-in-micro strategy to tackle the burden of pulmonary fungal diseases

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<sup>2</sup>Associate Laboratory i4HB - Institute for Health and Bioeconomy, Faculty of Pharmacy University of Porto

<sup>3</sup>LAQV-REQUIMTE, Department of Chemical Sciences, Faculty of Pharmacy University of Porto

Pulmonary fungal infections are a global health concern due to the emergence of new pathogens, fungal resistance uprising, growing population of immunocompromised individuals and limited diagnostic resources. Nystatin is an antifungal drug with a narrow applicability in therapy due to its physical/chemical instability, systemic toxicity, and low aqueous solubility/permeability<sup>1</sup>. Nonetheless, nystatin remains an affordable option which depicts high efficacy, and offers a broad action spectrum against overlooked fungal infections associated with mortality rates of up to 95% (cryptococcosis, candidiasis, aspergillosis, mucormycosis, blastomycosis, fusariosis and histoplasmosis)<sup>2</sup>.

Various strategies were devised to maximize nystatin's potential whilst addressing its main shortcomings. Firstly, nystatin-loaded nanoemulsions were developed to surpass its instability and solubility issues. A response-surface methodology permitted the methodical production of thermodynamically stable self-nanoemulsifying drug delivery systems (SNEDDS) which suffered no significant alterations for up to 6 months in terms of pH ( $3.07 \pm 0.1$ ), mean particle size ( $226 \pm 37$ nm), polydispersity index ( $0.282 \pm 0.04$ ), zeta potential ( $-42.2 \pm 0.1$ mV) and encapsulation efficiency ( $99.62 \pm 2.9\%$ ). Calorimetry analysis confirmed successful encapsulation of nystatin and a controlled release pattern of  $24.9 \pm 1\%$  release over 48 hours was observed, following zero-order kinetics. MTT cytotoxicity assays were performed on L929 and THP1 cells, revealing 70% viability for the SNEDDS until at least 24 and 8  $\mu$ g/ml, respectively. Flow cytometry confirmed nanoparticles internalization by macrophages.

Secondly, this optimized nanoemulsion was incorporated into a sodium alginate carrier through a microencapsulation technique. A computational tool (LabMate.ML) based on an adaptive machine-learning algorithm was applied to expeditiously select the best experimental parameters. With that, microparticles with a median microparticle size of  $12.35 \pm 0.8$  $\mu$ m were obtained. Additional experiments are underway to ensure favorable encapsulation, cytotoxicity profile, and drug release.

The development of these polymeric microcapsules containing nystatin-loaded SNEDDS aims to enable effective nose-to-lung delivery by means of a dry powder inhaler. Further research is required to validate the reported encouraging findings.

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**Biography:**

Filipa Sousa holds a master's degree in Pharmaceutical Sciences from Porto's University since 2017. From 2018 to 2021, she worked as a Data Manager at the National Association of Pharmacies, focusing on drug interactions analysis. Currently pursuing her PhD in Pharmaceutical Technology at UCIBIO- REQUIMTE, she aims to develop nano-in-micro formulations for neglected fungal diseases. She has also worked as an invited teaching assistant and e-learning tutor. She frequently participates in international conferences, authors scientific and journalistic articles and supervises undergraduate students. She does volunteer work for the Red Cross and for an extracurricular activities school. She loves traveling and reading.

**ACKNOWLEDGMENTS:**

This work was supported by the Foundation for Science and Technology, I.P. (FCT), Portugal, through grant reference 2020.05884.BD, and by the Applied Molecular Biosciences Unit – UCIBIO, which receives financial support from Portuguese national funds (FCT/MCTES, Fundação para a Ciência e Tecnologia and Ministério da Ciência, Tecnologia e Ensino Superior) through grant UIDB/04378/2020.

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## Magneto-plasmonic nanoparticles for non-toxic biomarker detection

Yevhenii Morozov<sup>1,\*</sup>, Anatoliy Lapchuk,<sup>2</sup> Ivan Gorbov,<sup>2,3</sup> Alexander Prygun,<sup>2</sup> Mykola Borysenko,<sup>4</sup> Jakub Dostalek<sup>5</sup>

<sup>1</sup>AIT-Austrian Institute of Technology, Vienna, Austria

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<sup>3</sup>University of Nottingham, Nottingham, UK

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We present our efforts to develop a novel non-toxic method for diagnostic biomarker extraction and concentration from biofluids, employing magneto-plasmonic nanoparticles.<sup>1</sup> The method utilizes magnetic nanoparticles of a few nanometers bearing molecular traps for biomarkers on their surface, along with larger magnetic nanoparticles for catching smaller ones in a strong magnetic field gradient. The interference of an external permanent gradient magnetic field with the magnetic field of large nanoparticles enables the capture of small magnetic nanoparticles from their trajectories in a fluid. A magnetic system based on multiple blocks of magnets with alternative orientations produces a strong gradient magnetic field over the fluid surface, allowing for efficient nanoparticle concentration without direct contact with the liquid. Theoretical analysis and mathematical simulations confirm the feasibility of this method, indicating fast and robust biomarker extraction and concentration, thereby enhancing sensitivity in biomarker detection. Experimental validation supports the effectiveness of the magnetic system in concentrating magnetic nanoparticles, aligning with the mathematical predictions.<sup>2</sup> This approach holds promise for developing advanced biosensors and diagnostic tools with improved sensitivity and selectivity. In addition, these results may be helpful in the development of microfluidic particle sorting technologies.

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### Biography:

Yevhenii Morozov earned his Ph.D. in Electrical Engineering from the National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute" in 2016. He completed postdoctoral research at Zhejiang University of Technology (China) and the Austrian Institute of Technology (Austria), supported by an Austrian Science Fund (FWF) Lise Meitner fellowship. Currently a Scientist at the Austrian Institute of Technology, his work focuses on diagnostic biosensor technologies and photonic integrated circuits (PICs) for optical coherence tomography. his research interests include plasmonics, biosensing, graphene-based metamaterials, PICs, hydrogels, and silica surface modification, to name a few.

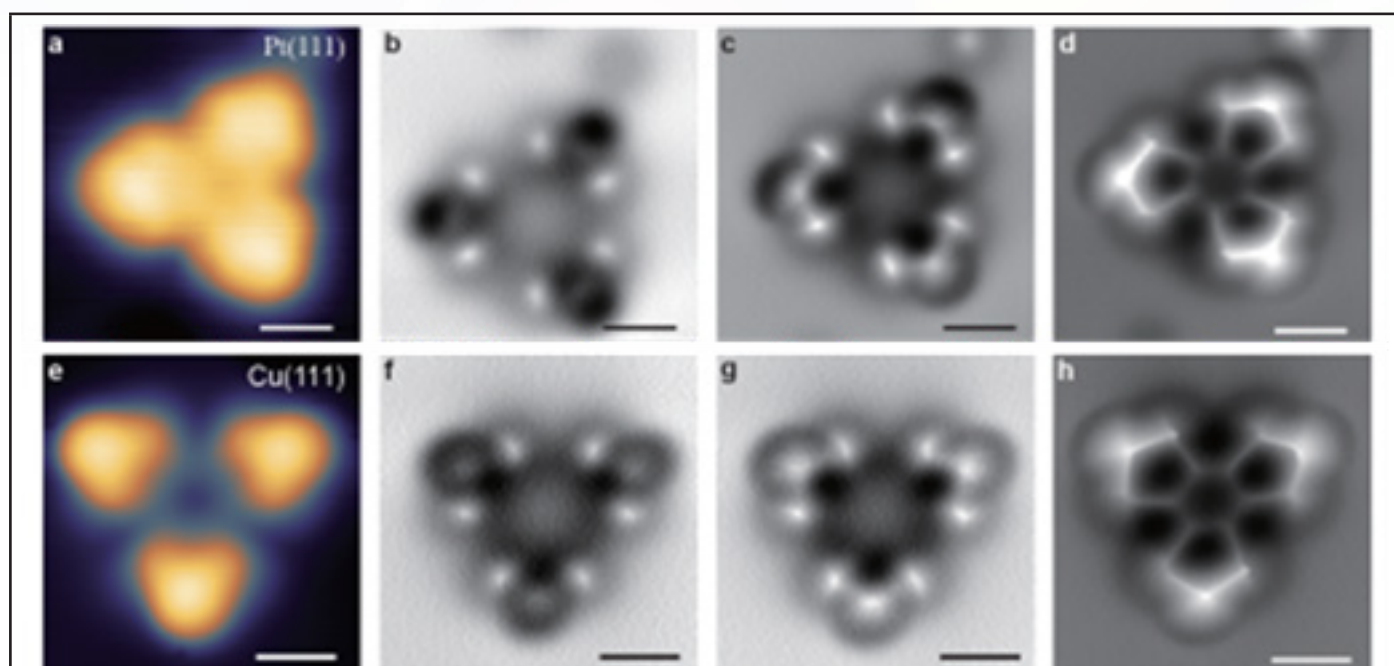
## Identifying a critical nucleus for ice nucleation on hydrophilic and hydrophobic surfaces

Pengcheng Chen, Nan Yao\*

*Princeton Materials Institute, Princeton University, Princeton, NJ 08540-8211, USA*

Water has long served as a critical topic in science and technology thanks to its ubiquitous existence in daily life. Water/solid interfaces are essential to an incredible range of everyday phenomena and technology developments, including wetting, corrosion, heterogeneous catalysis, environmental and atmospheric chemistry, biological science, and astrophysics. Studies of surface-supported water clusters provide a means to obtain a rigorous molecular scale description of the initial stages of the above processes.

here, we report a direct structural determination of the water clusters at the initial stages of ice nucleation on close-packed metal surfaces, represented by hydrophilic Pt(111) and hydrophobic Cu(111) surfaces using a combination of scanning tunneling microscopy (STM) and noncontact atomic force microscopy (NC-AFM). Real-space identification of the atomic structure of water clusters with precise information on the position of oxygen atoms and O-H bond orientation can be achieved using NC-AFM with a terminated tip. A series of hydrated clusters consisting of conjugated hexagon, pentagon, and heptagon rings were structurally identified through the atomically resolved NC-AFM images. We found similar structural motifs of water on both Pt(111) and Cu(111) surfaces, indicating the presence of universal starting nuclei at the initial ice growth stage on the terrace of wetting and non-wetting surfaces. Combined with first-principles density functional theory calculations, a critical nucleus comprising 15 water molecules has been identified, whereas further ice growth bifurcates to form two-dimensional (three-dimensional) layers on hydrophilic (hydrophobic) surfaces. A rigorous molecule-scale description of the initial stages of heterogeneous water nucleation is proposed.





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SPM characterization of water clusters with threefold symmetry on Pt(111) and Cu(111) with a CO-terminated tip and the corresponding structural models. a,e, Constant-current STM images of water clusters on Pt(111) and Cu(111). b-d, Constant-height AFM ( $\Delta f$ ) images of water cluster with threefold symmetry on the Pt(111) surface at tip heights of +30 pm (b), +10 pm (c), and -20 pm. (d). f-h, Constant-height AFM ( $\Delta f$ ) images of water cluster with threefold symmetry on the Cu(111) surface at tip heights of +30 pm (f), +10 pm (g), and -40 pm (h). Scale bars: 0.5 nm.

### **Biography:**

Professor Nan Yao is a leading scholar in materials characterization for interdisciplinary research. Yao is the founding director of Princeton's Imaging and Analysis Center. As a teacher, he is an eleven-time teaching award recipient at Princeton University. As a scientist, he has published two books and over 300 scientific articles with notable contributions, including the co-discovery of the first natural quasicrystal. This finding has revolutionized the science of natural crystal chemistry by identifying the third form of solid besides crystalline and non-crystalline. He is a fellow of the Microscopy Society of America, the Royal Microscopical Society, and the American Association for the Advancement of Science.

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## Low-cost point of care technology for personalized medicine

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<sup>1</sup>Department of Biomedical Engineering, Texas A&M University, USA

<sup>2</sup>Center for Remote Health Technologies and Systems, Texas A&M Engineering Experiment Station, USA

Portable diagnostic technologies are gaining more interest with the advancements in micro- and nano-fabrication. Cardiovascular diseases (CVDs) are one of the leading causes of death worldwide and reliable and accurate diagnostic tools with simple sample preparation steps are essential for screening of cardiovascular biomarkers at the point of care for early diagnosis of CVDs. Among the CVDs, blood thinning medicine, warfarin, is widely used to prevent coagulation and its prescribed dose levels deviates with the changes in the food diet and potassium intake, requiring the patient to make more frequent hospital visits to carry out related coagulation level tests by the clinicians. Here, we present a low-cost smartphone based device to screen blood coagulation levels at the point of care. The device does not require an external lens and not require a specific brand smartphone. We validated the performance of the device using ~50 clinical blood samples and control samples, achieving 90% overall accuracy. With its versatility and accessibility, this device could be a useful analytical tool for screening blood coagulation levels.

### Biography:

Dr. Hatice Ceylan Koydemir is a tenure-track Assistant Professor at Texas A&M University in the Department of Biomedical Engineering, a member of the Texas A&M Engineering Experiment Station Center for Remote Health Technologies and Systems, and a member of the NSF-funded ERC Precise Advanced Technologies and Health Systems for Underserved Populations (PATHS-UP). Dr. Koydemir is the Director of the Integrated Biomedical Sensing and Imaging Laboratory of Texas A&M University, and her research interests are in the area of integrated devices, and machine learning approaches, including mobile microscopes, MEMS-based biosensors, micro-fabrication technologies, and wearables for point-of-care analysis. She has co-authored more than 150 peer-reviewed publications in major scientific journals and conferences and holds seven issued/filed patent applications. Dr. Koydemir is a member of the SPIE, Optica, and BMES, as well as a senior member of IEEE.

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## Development of intelligent particles to prevent dental caries.

Yanping He,<sup>1</sup> Richard Bright,<sup>2</sup> Krasimir Vasilev,<sup>2</sup> and **Peter Zilm** <sup>1\*</sup>

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<sup>2</sup>College of Medicine and Public Health, Flinders University, Bedford Park SA 5042, Australia

Dental caries is one of the most prevalent non-communicable diseases worldwide, mediated by a multispecies biofilm that consists of high levels of acidogenic bacteria which ferment sugar to acid and cause teeth demineralization<sup>1</sup>. Current treatment practice remains insufficient in addressing 1) rapid clearance of therapeutic agents from the oral environment 2) destroying bacteria that contribute to the healthy oral microbiome. In addition, increasing concerns over antibiotic resistance calls for innovative alternatives<sup>2,3</sup>. In this study, we developed a pH responsive nano-carrier for delivery of polycationic silver nanoparticles<sup>4</sup>. Branched-PEI capped silver nanoparticles (BPEI-AgNPs) were encapsulated in a tannic acid- Fe (III) complex-modified poly(D,L-lactic-co-glycolic acid) (PLGA) particle (Fe(III)-TA/PLGA@BPEI-AgNPs) to enhance binding to the plaque biofilm and demonstrate “intelligence” by releasing BPEI-AgNPs under acidic conditions that promote dental caries. The constructed Fe(III)-TA/PLGA@BPEI-AgNPs (intelligent particles) exhibited significant binding to an axenic *Streptococcus mutans* biofilm grown on hydroxyapatite. Ag<sup>+</sup> ions were released faster from the intelligent particles at pH 4.0 (cariogenic pH) compared to pH 7.4. The antibiofilm results indicated that intelligent particles can significantly reduce *S. mutans* biofilm volume and viability under acidic conditions. Cytotoxicity on differentiated Caco-2 cells and human gingival fibroblasts indicated that intelligent particles were not cytotoxic. These findings demonstrate great potential of intelligent particles in the treatment of dental caries.

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## Biography:

Associate Professor Zilm is an academic member of the Adelaide Dental School at the University of Adelaide, Australia. He leads the Translational Research in Oral Health Science research group that investigates the translation of basic research to improve oral health. His research focus is nano-materials science and oral microbial biofilm/microbiomes. He has also developed numerous multidisciplinary collaborations which contribute to his multidisciplinary approach to research. He has received research funding from the NHMRC; The Australian Dental Research Foundation and industry (Nakao and Colgate). He received the Innovation in Oral Care award from the International Association for Dental research in 2023.

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**Intranasal administration of Pt(IV)-Based nanostructured coordination polymers for glioblastoma therapy**

**Fernando Novio**<sup>1\*</sup>, Ramiro Pérez-Becher<sup>1,2</sup>, Adrià Marañón Gràcia<sup>1,2</sup>, Roger Gòmez herrera<sup>2</sup>, Daniel Ruiz Molina<sup>2</sup>, Paula Alfonso Triguero<sup>2,3</sup>, Julia Lorenzo<sup>3</sup>.

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<sup>2</sup> *Catalan Institute of Nanoscience and Nanotechnology, CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain.*

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Glioblastoma multiforme (GB) is the most aggressive and frequent primary malignant tumor in the central nervous system (CNS), with unsatisfactory and challenging treatment nowadays that includes surgical resection followed by chemotherapy and radiotherapy. In this scenario few drugs (i.e. temozolomide) have demonstrated a significant success, as the blood brain barrier (BBB) still restricts its uptake when they are intravenously administered, thus limiting the therapeutic options [1]. Therefore, enormous efforts are being devoted to the development of novel nanomedicines and administration routes to cross or evade the BBB and specifically target the cancer cells reducing systemic concentration of drugs and, hence, side effects.

Cisplatin has been considered as a second-line therapeutic due to the restricted local bioavailability, lack of selectivity, and severe adverse effects. However, the use of Pt(IV) prodrugs open new challenges in the treatment of GB due to their therapeutic efficacy and limited systemic toxicity [2]. We propose a novel family of nanostructured coordination polymer made of a Pt(IV) prodrug, derived from cisplatin, that presents a notable in vitro therapeutic effect in GB cell lines (GL261). Moreover, intranasal administration route was employed to evaluate the anticancer efficacy in orthotopic GB murine models showing excellent in vivo biodistribution and tolerability [3,4].

The objective is to produce novel nanoformulations with improved lipophilicity and passive diffusion, promoting intracellular accumulation, while reducing toxicity and optimizing the concomitant treatment of chemo-/radiotherapy. Results gathered in this work in vivo, and the possibility to develop nanoformulations containing a combination of synergic drugs, open a future path for investigation of platinum derivatives for brain tumor treatment.

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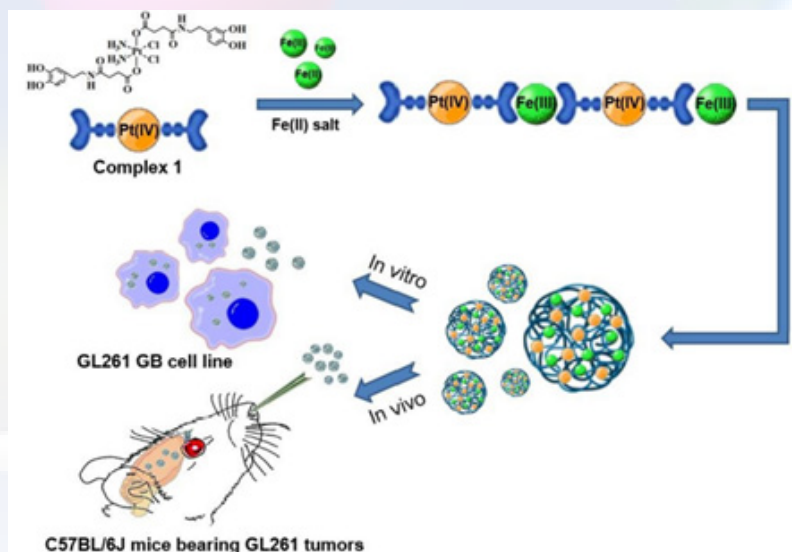


Figure 1. Scheme of the Pt-Fe NCPs synthesis, and analysis of their therapeutic effect in vitro (GL261 cell line) and in vivo murine models (C57BL/6J mice bearing orthotopic GL261 GB tumors).

### Biography:

Dr. Fernando Novio is graduated in Chemistry from the University of Santiago de Compostela (USC). He obtained his PhD in chemistry (2007) in the Autonomous University of Barcelona (UAB). Then he moved to the Laboratoire de Chimie de Coordination (LCC) in Toulouse (France) for his postdoctoral stage (2008-2010), and from 2011 to 2021 he joined the Catalan Institute of Nanoscience and Nanotechnology (ICN2), as Senior Researcher. From 2022 he is Associate Professor in the Chemistry Department at UAB. his research subject is related principally to the technological and biomedical application of coordination polymer nanoparticles and other polymer-based nanoformulations.

## **A Comprehensive study of Gum Arabic/Chitosan Polyelectrolyte Complexes**

**Clémence Delmas\***, Florentin Michaud, Alain Durand and Jordane Jasniewski

*LIBio/LCPM Université de Lorraine, Nancy, FRANCE*

Electrostatic interactions among oppositely charged polysaccharides lead to interesting self-assembled systems with great potential for drug delivery applications<sup>1</sup>. These attractive electrostatic interactions result in the formation of various soluble or insoluble colloids such as complexes, complex coacervates and aggregates<sup>2,3</sup>. The stability and evolution of these complexes has not been studied thoroughly. This work aims to provide a clear definition of the various colloids and assess their stability over time.

We focused our study on electrostatic systems involving various molar mixtures of gum arabic and chitosan, two oppositely charged ionic polysaccharides. The experiments were conducted in acidic buffered media at a temperature of 20 °C keeping the same overall biopolymer concentration. The formation and stability of the systems were monitored for 28 days using dynamic light scattering, electrophoretic mobility measurement, turbidimetry measurement, and microscopy. In addition, the structure and morphology of the systems were studied via scanning and transmission electron microscopy and small angle x-ray scattering<sup>4,5</sup>.

Results showed that when charge equilibrium was reached, complete phase separation occurred, forming complex coacervates. In the pre-charge equilibrium (with an excess of gum arabic) soluble complexes were formed; eventually, their coalescence led to the formation of coacervate-like structures. However, in the post-charge equilibrium (with an excess of chitosan) complexes were formed, and microscopic observations suggested that their coalescence led to more aggregated structures. The soluble complexes were stable over 3 days before starting to undergo coalescence and sedimentation. The sizes of complex coacervates increased immediately and continuously after their formation.

This work opens the way to further studies about the preparation of specific types of colloids according to the followed procedure and their potential use for encapsulation and release of active molecules taking the opportunity of their particular morphology

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**Biography:**

Clémence Delmas is a PhD student working on complex coacervation of polysaccharides at both the Engineering Laboratory of Biomolecules (LIBio) and the Laboratory of Physical- Chemistry of Macromolecules (LCPM) based in Nancy (FRANCE). She graduated from the National graduate school of chemistry in Montpellier where she specialized in material chemistry and she is very passionate by encapsulation processes.

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## The structure and properties of the high temperature recovered nanoscale carbon

**Akaki Peikrishvili,\*** Roin Chedia, Lali Gurchumelia, Archil Mikeladze, Marqalita Darchiashvili, Bagrat Godbadze

*Ferdinand Tavadze Institute of Metallurgy and Materials Science, Tbilisi, 0186, Georgia*

Two stage method to recover nanoscale carbon from plastic (PET) waste in overheated vapor environment including low-temperature pyrolysis of waste at the first stage in control environment (CO<sub>2</sub> & Argon) and followed high temperature thermal/chemical treatment (around 900°C) in vapor environment was developed.

The investigation showed that application of two stage combined method of pyrolysis allows essentially to reduce loses of char and increases output of nanoscale carbon after final, high temperature second stage processing in overheated water vapor environment.

The initial treatment in vapor (up to 700°C) activates the pyrolysis process increasing the primary reactions of hydrocarbon decomposition. At first stage the release of gases increases and the main part of which is extracted as a liquid fraction - pyrolytic oil and reminder amorphous coal containing different organic/inorganic impurities. At second stage after increasing of the temperature above 700°C and simultaneously feeding of overheated vapor, the increasing the rates of side reactions and full decomposition pyrolytic reminders takes place. As a result, the loosening of the formed carbon aggregates occurs with followed formation of the highly dispersed, nanoscale carbon particless.

As investigation showed (including SEM observation) the characteristics of obtained nanoscale carbon changes in wide range depending from processing conditions (vapor temperature, vapor feeding rate, processing period etc.) and may reach to 1000 m<sup>2</sup>/g (BET surface area) and 98.7% (purity) respectively. The resistivity of obtained recovered carbon may be reach 1-1.3 OM.SM<sup>-1</sup>.

This work was supported by Shota Rustaveli National Science Foundation of Georgia – SRNSFG (Grant number NFR-22-4275).

### Biography:

Akaki Peikrishvili (PhD, Dipl. Engineer) is a head of laboratory of Tavadze Institute of Metallurgy and Materials Science. 2001-2018 the coordinator and head of the Office of STCU ([www.stcu.int](http://www.stcu.int)) in Georgia

Dr. Peikrishvili's has led and participated in more than 200 international scientific projects and award contracts, including projects with BNL and LLNL of DOE USA and US Army Research Laboratory. He is a frequent speaker at international conferences and symposiums. Dr. Peikrishvili is Certified Expert on explosive engineering. He has published more than 120 scientific articles in Georgian and International journals/proceedings in the field of materials science and nanotechnology.



## Development of 3D-printed breast cancer models for the evaluation of anticancerous systems

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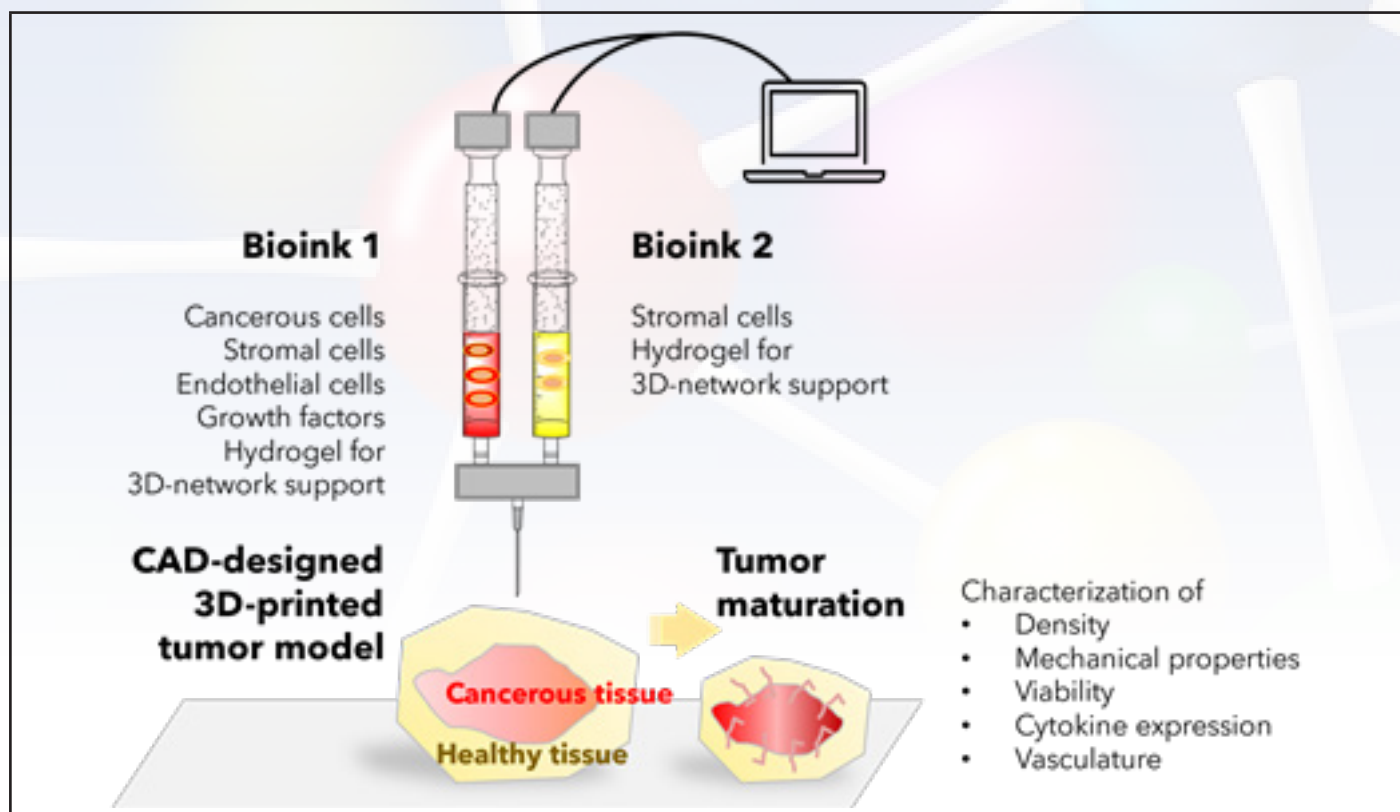
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Highly cytotoxic drugs, essential in cancer chemotherapy, show important side effects due to their distribution across healthy tissues.<sup>1</sup> Thus, their focalization within tumors remains one of the most difficult challenges. The use of drug delivery systems such as nanoparticles or microparticles can importantly decrease their diffusion, importantly improving the safety and efficacy.<sup>2</sup>

Drug testing in 2D cell cultures only partially reflects the response in vivo. Instead, 3D-printing technology now permits the creation of synthetic tissues, resembling a real biological tissue to test anticancer drugs/systems in a more accurate way than in 2D, yet much cheaper, faster, reproducible, and with many less bioethical implications than in vivo.<sup>3</sup>

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In this project, we are using 3D-bioprinting to develop breast cancer models using alginate and gelatin mixtures as the bioink. An extensive screening let us select the most promising ones and performed several rheological analyses to understand their mechanical properties.<sup>4</sup> With this, we have established the optimum printing parameters such as temperature, holding time, and printing pressure, achieving stable structures with micrometric resolution. The bioinks showed very good biocompatibility, proving the feasibility of the tumor model being developed.

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**Biography:**

David Limón carried out his PhD on the development of nanomaterials for drug delivery in skin diseases. Since 2017, he has been a Postdoctoral Researcher in institutions such as the University of Barcelona (Spain), Northwestern University (USA), or University College London (UK). his areas of expertise include the synthesis, functionalization, characterization, and efficacy evaluation of supramolecular hydrogels, nanoparticles, and silicon microparticles (microchips).

He has published 20 articles in peer-reviewed journals, has supervised 9 students (exchange students/ BSc/ MSc), and has participated as a Jury of 2 MSc and 2 PhD students.

Since 2017 he is an Assistant Professor at the University of Barcelona.

Currently, he is PI funded by La Caixa Foundation through a Junior Leader Fellowship at NOVA School of Science and Technology in Lisbon.

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**Preparation and characterization of multifunctional Ag-SiO<sub>2</sub>-TiO<sub>2</sub> nanocoatings on NiTi SMA**

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**Presenting author:**

Karolina Dudek

To functionalize the NiTi shape memory alloy, its surface was modified by creating Ag-SiO<sub>2</sub>-TiO<sub>2</sub> nanocomposite layers. A stable colloidal suspension with a concentration of 0.1 wt. % was prepared using chemically synthesized nanocomposite in 75% ethanol, achieving a Zeta potential of -21.9 mV. Anaphoretic deposition was then performed at a voltage of 40 V for various deposition times ranging from 1 to 10 minutes. Scanning electron microscopy revealed that the deposition parameters significantly influenced the morphology of the produced coatings, while Raman spectroscopy provided detailed structural characterization. The coatings exhibited structural variations depending on the deposition conditions.

To enhance adhesion between the substrate and the electrophoretically deposited ceramic coatings, heat treatment was applied. Parameters for this treatment were selected using high-temperature microscopy, dilatometry, and thermogravimetry. The tests indicated that to avoid shrinkage of the coating, the heat treatment temperature should not exceed 800 °C. This treatment resulted in significant structural and morphological changes in the deposited coatings. Layers with a completely different structure compared to the starting materials and those produced by electrophoretic deposition were obtained. The heat treatment severely altered the nanocomposite structure, resulting in novel layers characterized by high reactivity.

Acknowledgement: This research was funded by the National Science Center in Poland (NCN), grant number 2020/39/D/ST5/01531.

**Biography:**

Researcher at the Łukasiewicz Research Network - Institute of Ceramics and Building Materials in Krakow, Centre of Refractory Materials in Gliwice, Poland. I hold a PhD in Material Engineering from the Institute of Materials Science at the University of Silesia in Katowice. My scientific interests encompass a broad spectrum of materials science, with a particular focus on ceramic materials (especially refractory materials), nanomaterials, surface engineering and biomaterial surface modification

# Posters

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**The Study of Sintered Wick Structure of Heat Pipes with Excellent Heat Transfer Capabilities**

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A sintered wick was formed in a heat pipe through the process of sintering a mixture of copper powder with particle sizes of  $100\mu\text{m}$  and  $200\mu\text{m}$ , mixed with a pore-forming agent. The heat pipe's thermal resistance, which affects its heat transfer efficiency, is determined during manufacturing according to powder type, thickness of the sintered wick, and filling rate of the working fluid. Heat transfer efficiency was then tested at various inclination angles ( $0^\circ$ ,  $45^\circ$ ,  $90^\circ$ ) to evaluate the performance of heat pipes. Regardless of the filling amount and test angle, the  $200\mu\text{m}$  copper powder type exhibited superior heat transfer efficiency compared to the  $100\mu\text{m}$  type. After analyzing heat transfer performance at various filling rates between 20% and 50%, it was determined that the heat pipe's optimal heat transfer capability occurred at a working fluid filling rate of 30%. The width of the wick was directly related to the heat transfer performance.

## **Au(I)-TADF Emitters for High Efficiency Full-Color Vacuum-Deposited OLEDs and TADF-Sensitized Fluorescent OLEDs with Ultra high Brightness and Prolonged Operational Lifetime**

Rui Tang, Shuo Xu, Lili Du, Faan-Fung Hung, Tsz-Lung Lam, **Gang Cheng**,\* Kam-Hung Low, Qingyun Wan, Siping Wu, Yong Chen, and Chi-Ming Che

*Department of Chemistry, The University of Hong Kong*

here we report a class of structurally simple, efficient, and operationally stable Au(I)-TADF (TADF = thermally activated delayed fluorescent) materials based on a carbene-metal-amide (CMA) molecular scaffold comprising of sterically bulky N-heterocyclic carbene (NHC) ligands with N-heterocyclic  $\pi$ -annulation. These CMA(Au) emitters, supported by pyridine-, pyrazine- or quinoxaline-fused NHC ligand, are thermally stable (decomposition temperature of 302–348 °C), adopt co-planar or uncommon orthogonal geometry between the carbene and amide ligands, and show strong blue to deep red TADF emissions (468 – 666 nm) from a thermally-equilibrated singlet ligand-to-ligand-charge-transfer ( $^1LL'CT$ ) excited state with emission quantum yield of 0.63 – 0.99 and fast radiative decay rate constants of  $0.68 - 3.2 \times 10^6 \text{ s}^{-1}$  in thin film samples at room temperature. The effect of increasing py-extension and number of N-substitution of the NHC backbone as well as orthogonal molecular geometry are similarly manifested in the reduction of both the singlet-triplet energy gap and the  $S_1$  transition dipole moment. The vacuum-deposited Au(I) devices displayed superior electroluminescence characterized by ultrahigh brightness up to  $300,000 \text{ cd m}^{-2}$  and external quantum efficiencies up to 26.2% with roll-offs down to 2.6 % at  $1000 \text{ cd m}^{-2}$  alongside record-setting device lifetimes ( $LT_{95}$ ) up to 2082 h among reported TADF OLEDs.

### **Biography:**

Dr. Gang Cheng, a Research Assistant Professor in the Department of Chemistry at the University of Hong Kong, received his Ph.D. degree from Jilin University in China. He has published over 100 peer-reviewed papers and has an h-index of 41.

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**The large pore-size characteristics on the electric double-layer capacitance for high voltage by <sup>19</sup>F-NMR: A quantitative evaluation**

**Joo-Il Park\***

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Electrical bilayer capacitors (EDLCs) utilize the adsorption and desorption of dielectric ions on porous material surfaces to provide long lifespan and high power density. However, their electrical capacities tend to decrease when used at high voltages. The present study quantitatively assessed how the large pore size of activated carbon (AC) affects the electrical capacitance of electrical bilayer capacitors at various voltages. KOH activation and spherical phenol resins (SPRs) were used to achieve high precision surface areas. The pore structure was characterized using adsorption system analysis and scanning tunneling microscopy (STM). The electrochemical properties of ACs were evaluated by cyclic voltammetry (CV), battery testing, and electrochemical impedance spectroscopy (EIS). In addition, solid state <sup>19</sup>F-NMR measured the dissolved ion concentration of ACs. As a result of analyzing ACs with well-developed micropores and intermediate pore structures through KOH activation, ACs with small amounts of mesopores exhibited a non-static capacity of 30.35 F/g at a voltage of 2.7 V, significantly lowering to 20.93 F/g at a high voltage of 3.3 V. On the other hand, the intermediate pore-rich AC showed 40.77 F/g at 2.7 V and 38.22 F/g at 3.3 V, confirming that the intermediate pore structure served as a buffer to mitigate capacity reduction at high voltages. These intermediate pores can contribute to capacity retention by acting as a buffer space for mobility and diffusion of dissolved ions at high voltages.

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## Cooling Crystallization of L-Glutamic Acid for Crystalline control

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*Department of Chemical & Biological Engineering, Hanbat National University, Daejeon, 34158, Republic of Korea*

In this study, cooling crystallization was performed for crystalline control of L-Glutamic acid (LGA).  $\alpha$ -form and  $\beta$ -form are known as the crystalline types of LGA. Industrially preferred crystalline types are  $\alpha$ -form, as they offer advantages in downstream processes such as drying and filtration. The primary distinction between the two crystalline types lies in the aspect ratio of the crystals, with  $\alpha$ -form being isotropic and  $\beta$ -form being needle-like. This study controlled the aspect ratio of the crystals according to the cooling conditions and observed their shapes using an optical microscope. Furthermore, it investigated the differences that arose during the downstream drying process.  $\alpha$ -form seed and  $\beta$ -form seed were utilized for seeding crystallization. With  $\alpha$ -form seed, the aspect ratio improved under conditions of low supersaturation and slow cooling rates, whereas  $\beta$ -form seed exhibited the opposite effect. In addition, it was confirmed that the shape of the cake formed by stacking on the filter after filtration varies depending on the crystal form of  $\alpha$ -form and  $\beta$ -form. This difference affects which mother liquor is removed during the filtration process. As a result, it was possible to improve the aspect ratio of the crystal by controlling the supersaturation and cooling rate. Additionally, the study confirmed differences in the drying rate and mother liquor content between  $\alpha$ -form and  $\beta$ -form.



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**Physical restoration of waste artificial graphite through heat treatment and recycling as an anode material for secondary batteries**

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*Department of Chemical & Biological Engineering, Hanbat National University, Daejeon, 34158, Republic of Korea*

The manufacturing process of artificial graphite involves considerable energy use and environmental burden, but the recyclability of this resource has not yet been fully explored. Developing a method of recycling waste artificial graphite to manufacture a high-performance secondary battery anode material can contribute to the improvement of the environmental sustainability of the secondary battery industry. This study effectively recovered and strengthened the physical and chemical properties of waste artificial graphite by applying a high-temperature heat treatment technique (above 1200°C). Defects inside the base surface of the carbon network under heat field are effectively suppressed, so that cross-sectional carbon atoms can easily combine with other carbon atoms to form larger p-bonds, and extra energy is released due to high activity. In addition, oxygen defects inside the carbon network are also replaced by carbon atoms, and unstable carbon atoms are activated through heat treatment. After that, the disordered structure is converted into an ordered layer structure. All samples subjected to various temperature treatments were measured by XRD and Raman spectroscopy to confirm the interplanar spacing ( $d_{002}$ ) and crystallinity ( $I_D/I_G$ ). Electrochemical tests were performed to confirm the resilience of graphite. The reversible capacity of the heat-treated recycled anode material was evaluated at 0.1C, and the specific capacities at various current densities were compared. As the recovered graphite increased from 1C to 5C, the specific capacity decreased sharply, while the specific capacity gradually decreased at 7C. Recycled anode materials treated at 2000°C not only exhibited interplanar spacing and crystalline values similar to those of commercial graphite, but also confirmed the recyclability as a anode material for secondary batteries through comparison of discharge capacity and initial efficiency.

**Biography:**

Currently pursuing a Master's degree in the Department of Chemical & Biological Engineering at Hanbat National University, Yujin Kim is deeply engaged in research within the fields of energy and environmental catalysis. her focus is particularly on exploring the potential for recycling waste artificial graphite into anode materials for secondary batteries. She has already presented her research on this topic at an academic conference and continues to conduct sustained research in this area. Yujin is driven by a vision to contribute to sustainable energy solutions through innovative recycling methods.

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## Improving Bee Living Conditions through Composite Ecological Thermal Insulation

**Wrześniewska-Tosik K.**<sup>\*1</sup>, Mik T.<sup>1</sup>, Wesołowska E.<sup>1</sup>, Kowalewski T.<sup>1</sup>, Walisiak D.<sup>1</sup>, Pałczyńska M.<sup>1</sup>, **Wietecha J.**<sup>1</sup>, Górecki S.<sup>2</sup>

<sup>1</sup> LUKASIEWICZ Research Network- Lodz Institute of Technology, Lodz, Poland

<sup>2</sup> Intelligent Hives Sp. z o.o., pl. Kościuszki 6a, 99-200 Poddębice, Poland

Intelligent Hives project integrates the Internet of Bees (IoB) system with electronic hardware, middleware, and a presentation module for real-time bee colony monitoring. Its standout feature is an ecological thermal insulation cover, made from a nonwoven blend of sheep's wool and chicken feather waste, enhancing hive durability and bee health. Innovative, composite nonwovens were manufactured by needle punching and were carried out on an experimental line held by Łukasiewicz- Lodz Institute of Technology which is configured with the following devices: carding machine cutter, an aerodynamic moulding machine, fleece compacting rolls, a conveyor, a needle-punching machine and a coiler.

Tested in harsh conditions, these covers proved to significantly improve bee survival and activity. The system, easily implemented and AI-supported for data analysis, marks a sustainable advancement in beekeeping, optimizing hive conditions and bee health management.

The Intelligent Hives system demonstrated remarkable effectiveness in bee colony management. During swarming, the system maintained optimal brooding temperatures (33-36°C) irrespective of external conditions. In winter, the central hive temperature was consistently around 25°C. The system's sensors could track colony development stages by observing temperature variations.

For instance, a rise in the upper hive temperature indicated increased food consumption, crucial for colony survival during colder months. The experiment also validated the system's wireless sensor-cloud integration, ensuring data archiving and user-friendly presentation for beekeepers. Additionally, winter studies highlighted the significant impact of the ecological thermal insulation cover. Comparisons between covered and uncovered hives in February 2023 showed a notable average temperature difference of 5.4°C, reaching up to 9°C on sunny days due to the cover, which enhanced internal warming. This proved the cover's efficacy in improving bee colony conditions during overwintering.

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**Biography:**

Assistant Professor Krystyna Wrześniewska-Tosik is head of the Composite Materials Research Group. Krystyna Wrześniewska-Tosik has experience in research on biopolymers - modification, processing and application, in particular keratin from waste materials (feathers, wool). She has conducted research, development and implementation work in 85 national and international projects. She is the author and co-author of 35 patents and 4 patent applications, 43 scientific publications, including the monographic study "Modern composite materials containing keratin fibres", related to biopolymers and environmentally friendly technologies. She presented her research results at numerous scientific conferences (more than 90) and at invention competitions (i.a. Brussels, Paris, Taipei, London, Istanbul, Bangkok, Valencia, Barcelona, Kuala Lumpur, Zagreb).

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**ZnO Transistors Fabricated by Atomic Layer Deposition Process at Low Temperature**

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<sup>4</sup>Peking University Shenzhen Graduate School, Shenzhen 518055, China

The Oxide semiconductor material and thin-film transistors (TFTs) have received intense attention in the next-generation semiconductor and displays field due to their desirable properties over silicon-based TFTs, including low processing temperature, good device performance, and high transparency in a visible range. The quality of transistors is needed to increase to meet the demands of large-area and high-resolution displays in the market. Tremendous efforts have been made in high-performance oxide TFTs research, including the development of new channel materials, the exploration of low-resistance ohmic contacts, and the introduction of high-k dielectric materials as the gate insulator. Employing the high-k materials as the gate dielectric is an effective way to improve the subthreshold swing (SS) and reduce the operation voltage range. Al<sub>2</sub>O<sub>3</sub> is a promising gate dielectric in novel TFTs technologies because of its high relative permittivity and low leakage current with a wide- bandgap (6.6 eV). Recently, oxide TFTs based on atomic layer deposition (ALD) exhibit comparable characteristics to conventional deposition methods, such as magnetron sputtering and sol– gel method. ALD can produce large areas and high quality oxide thin films, including semiconductors, conductors, and dielectrics at relatively low temperatures, which makes it compatible with both glass and plastic substrates. This work was supported by the BJSAMT Project (SAMT-2022-PM02-14) and Shenzhen Science and Technology Innovation Committee under Grant KQTD 2020082011310-5004.

**Biography:**

Han Dedong received a Ph.D degree from Peking University and is working as a Research Professor in School of Integrated Circuits, Peking University. his research interests include new semiconductor materials and devices, flexible electronics, new thin film transistors, and nanotechnology. He has published more than 100 scientific papers and applied for more than 50 patents.

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## **Durable Triboelectric Nanogenerator on Coiled Head of Acupuncture Needle**

Saira Iqbal \*, Jinlian Hu

*Department of Biomedical Engineering, City University of Kowloon Tong, Hong Kong*

The synergy between Traditional Chinese Medicine (TCM) and modern technology continues to yield groundbreaking advancements, transcending traditional boundaries and opening new avenues for interdisciplinary exploration. This research investigates the innovative integration of acupuncture, a cornerstone of TCM, with triboelectric nanogenerators (TENG), an emergent energy harvesting technology.

Our study focuses on the transformation of acupuncture needles' coiled heads into multifunctional sensors capable of harnessing mechanical energy via the triboelectric effect. Through meticulous design and fabrication, we create a TENG sensor atop the acupuncture needle's coiled head, comprising layers of polydimethylsiloxane (PDMS) infused with multi-walled carbon nanotubes (MWCNTs), an insulating layer, and a conductive layer.

This integration enables the conversion of mechanical energy generated during acupuncture into electrical energy, facilitating self-powered electroacupuncture systems. Noteworthy attributes of the sensor include its high compressibility, durability, and sensitivity to mechanical stimuli, ensuring reliable performance in clinical settings.

Experimental validation demonstrates the sensor's efficacy in generating electrical power in response to mechanical stimulation, thus realizing the potential for real-time electroacupuncture data replication. This dual functionality not only enhances the therapeutic efficacy of electroacupuncture but also provides a sustainable energy source, fostering self-sufficiency in treatment processes.

By integrating ancient TCM principles with cutting-edge energy harvesting technology, our research heralds a paradigm shift in healthcare delivery. This convergence not only enhances therapeutic modalities but also fosters a deeper understanding of the synergies between traditional wisdom and modern innovation. Our findings underscore the transformative potential of interdisciplinary collaborations, paving the way for novel solutions that bridge the gap between tradition and progress in healthcare.

### **Biography:**

Saira Iqbal received her bachelor's degree (2016) in Mechatronics and Control Engineering from the University of Engineering and Technology, Lahore, Pakistan and her master's degree (2019) in Mechatronics Engineering from Harbin Institute of Technology, China. She is currently Ph.D. candidate under the supervision of Prof. Jinlian Hu at the School of Biomedical Engineering, City University of Hong Kong. Her research is focused on energy-harvesting devices and wearable electronics.

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**Temperature dependent phase transformation in Ag-SiO<sub>2</sub>-TiO<sub>2</sub> nanocomposites for multifunctional layer on Ni-Ti memory shape alloy.**

Jacek Podwórny<sup>1</sup>, Karolina Dudek<sup>1</sup>, Magdalena Kujawa<sup>1</sup>, Anna Gerle<sup>1</sup>, Anna Nowak<sup>2</sup>

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<sup>2</sup> Institute of Biology, Biotechnology, and Environmental Protection, Faculty of Natural Sciences, University of Silesia, Jagiellonska 28, 40-032 Katowice, Poland;

As part of the work, Ag-TiO<sub>2</sub>-SiO<sub>2</sub> nanocomposites were produced using chemical synthesis methods from pure substrates. The purpose of producing these nanocomposites was to develop powder precursors, which in further research were used to create multifunctional layers on the surface of Ni-Ti shape memory alloys. The ultimate purpose of these layers is to modify the surface of implants made of shape memory alloys. In order for the obtained Ag-SiO<sub>2</sub>-TiO<sub>2</sub> nanopowders to be used to produce functional coatings, their heat treatment is necessary to increase the adhesion of the coating to the substrate. To obtain the best results, the process should be carried out in a temperature range that does not cause excessive sintering of the layer, leading to the formation of cracks and delaminations. Experimental research techniques such as: high-temperature X-ray diffractometry, high-temperature microscopy and thermal analysis show phase transformations during heating of nanopowders. produced using different polymorphic forms of TiO<sub>2</sub> (rutile or anatase) and different proportions of the amorphous silica. The identified course of phase transformations and the mechanism of Ag release into the layer strongly depend on the polymorph of TiO<sub>2</sub>. The influence on this process results from the different behavior of both types of titanium oxide during the synthesis of the nanopowders, during which a layer of solid solution of (Ag,Ti)O<sub>2</sub> is formed on the surface of the anatase particles, which determines a different mechanism of Ag release into the layer than in the case of rutile of which such a layer does not form. To characterize the functional properties of the nanocomposites, their sintering temperature and dimensional changes during heating were determined. Sinterability tests revealed that the maximum annealing temperature should not exceed 850°C. This comprehensive analysis contributes valuable insights into the behavior of Ag-SiO<sub>2</sub>-TiO<sub>2</sub> nanocomposites under elevated temperatures, offering a foundation for their potential applications.

Funding: This research was funded by the National Science Center in Poland (NCN), grant number 2020/39/D/ST5/01531.



**Day-1  
Virtual**





## **An automated and accelerated computational framework to compute finite temperature properties including anharmonic effects in different property domains**

**Pinku Nath**<sup>\*1</sup>, Yuki Ide<sup>1</sup>, Jose. J. Plata<sup>2</sup>, Yasuhide Inokuma<sup>1,3</sup>, Masaharu Yoshioka<sup>1,4</sup>

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<sup>3</sup>*Division of Applied Chemistry, Faculty of Engineering, Hokkaido University, Kita 13, Nishi 8 Kita-ku, Sapporo, Hokkaido 060-8628, Japan*

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Accurately predicting the properties of solids at finite temperatures is a computationally intensive task. Calculating thermodynamic, mechanical, and thermal transport properties simultaneously can greatly increase the computational cost. Traditionally, different computational setups are required to predict these three types of properties or domains. Moreover, the information generated while computing one domain is generally not utilized in the other two. Besides the high computational cost, traditional methodologies often overlook the need for incorporating high-temperature corrections that stem from the anharmonicity of the material. To tackle these challenges, an automated and accelerated computational framework has been developed to enable the computation of finite properties of the three above-mentioned domains simultaneously. This new approach utilizes interdomain data efficiently and combines accelerated methodologies such as machine learning regression for the extraction of high-order force constants and the quasi-harmonic three-phonon method to reduce the computational cost without compromising accuracy [1-4]. Temperature-dependent phonons are included in the calculation to include strong anharmonic effects. The methodology can be used with either classical interatomic potential or DFT-based codes.

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**Biography:**

Education.

2004/00 B.S. Chemistry, Assam University, India

2006/04 M.S. Chemistry, Indian Institute of Technology Guwahati, India

2014/07 Ph.D. Chemistry, Indian Institute of Technology Kanpur, India with Prof. Madhav Ranganathan.

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**Atomic-scale cognition of c-Si/a-Si:H interface in high efficiency silicon heterojunction solar cells**

**Kun Zheng**

*Beijing University of Technology, China*

The crystalline silicon (c-Si)/a-Si:H heterojunction is a key factor in further SHJ efficiency improvement. In recent years, we have utilized advanced spherical aberration electron microscopy to focus on the microstructure of c-Si/a-Si:H heterojunction interfaces [1,2], revealing their structural characteristics at the atomic scale, achieving their in-situ structural evolution under appropriate external field loading and establishing the correlation between microstructure and macroscopic properties. High-density embedded nanotwins, detrimental to the device performance, were identified in the thin epitaxial layer between c-Si and a-Si:H for the first time [1], and a hybrid interface by tuning pyramid apex-angle were designed to improve c-Si/a-Si:H interfacial morphology in silicon solar cells [2].

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1. Qu, X.L.; et al. Identification of embedded nanotwins at c-Si/a-Si:H interface limiting the performance of high-efficiency silicon heterojunction solar cells. *Nature Energy* 2021 6,194–202.
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**Biography:**

ZHENG Kun is currently a full professor of Beijing University of Technology. He obtained his Ph D. in 2009, and his doctoral dissertation was awarded "National Excellent Doctoral Dissertation of China", he won 1st prize of "Beijing Municipality Science and Technology Award" (2016) and 2nd prize of "National Natural Science Award" (2020). He has published more than 100 SCI papers on international major journals and 1 academic book, including *Nature Energy*, *Nature Communications*, *Advanced Materials*, *EES*, *Nano Letters*, etc.

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**Capacitive Piezotronic Force Sensor with Ultra-Low Power for Next- Generation Sensory Memory System**

**Chao-Hung Wang**<sup>1,2\*</sup>, Yu-Liang Hsiao<sup>3</sup>, Chen Jang<sup>3</sup>, Yi-Miao Lin<sup>3</sup>, Jiu-Zhang Zheng<sup>1</sup>, Chuan-Pu Liu<sup>2,3</sup>

<sup>1</sup>*Miin Wu School of Computing, National Cheng Kung University*

<sup>2</sup>*Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University*

<sup>3</sup>*Department of Materials Science and Engineering, National Cheng Kung University*

The surge in Artificial Intelligence and the Internet of Things (AIoT) necessitates the creation of ultra-low-power solutions for forthcoming sensory memory system. This work introduces a specialized capacitive piezotronic force sensor for tactile sensing, ensuring ultra-low- voltage operation under nearly 0 reading bias conditions with consistent response across a broad voltage range. The inclusion of the near-sensor computation concept illustrates the future of sensory memory systems. By directly detecting capacitance changes induced by piezocharges, this sensor reflects perturbations in the effective depletion width, achieving ultralow power capability by eliminating the need to activate the Schottky diode initially. Its dynamic response showcases remarkable power efficiency and immunity to triboelectric interference, rendering it ideal for tactile sensing in robotics, prosthetics, and wearables. Moreover, these tactile signals, treated as time-series data, can be efficiently processed through the near-sensor computation technique with the energy-efficient Brain-like computing model, particularly employing spiking neural networks. This approach facilitates tasks like classification at an ultra-low power consumption. The study contributes valuable insights and design principles for the development of future ultra-low-power sensory memory system.

**Biography:**

Dr. Chao-Hung Wang, who earned his PhD in Materials Science and Engineering from NCKU in 2015, conducted R&D at Macronix Inc. (2015-2019) and received the LEAP scholarship at U.C. Berkeley (2019-2020). As an advisor to ANAFLASH Inc. under the Berkeley Science Fellow Program, he researched neuromorphic processors. Following LEAP, he worked at TSMC on interconnect metallization (2020-2021). Now an Assistant Professor at NCKU since August 2021, Dr. Wang specializes in non-volatile memory, novel memory devices, sensors, and future computing technology, with over 20 SCI and conference papers, 8 patents, and a notable citation count (682) and h-index (15).

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**Development of automotive quality high-strength steel microalloying principles to reduce production costs with keeping required mechanical performance**

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<sup>1</sup>Novolipetsk Steel, Lipetsk, Russia.

<sup>2</sup> I. Bardin Central Research Institute of Ferrous Metallurgy, Moscow, Russia

According to the study, optimal alloying systems were established to achieve the required mechanical properties, content of non-metallic inclusions (NI) and grain grade. Four heats of S355MC grade were produced and hot rolled according to EN 10149 in industrial environment of Novolipetsk Steel, in which the content of micro-alloying elements, Nb and Ti, varied.

Mechanical properties of samples with the Nb, Nb-Ti and Ti alloying systems meet the requirements of the regulatory documentation. A significant impact of Ti microalloying on dispersion and spheroidization of the sulfide component was revealed, which additionally confirms the benefits of adding titanium. The possibility of casting titanium microalloyed steel slabs right after niobium microalloyed steel slabs has been established.

When comparing the grain structure of experimental and comparative rolled products, a significant decrease in uneven grain size in cross section was noted. The grain size in the axial zone is larger than that at the surface in all samples of steel strips.

The obtained strength characteristics of automotive steel sheets microalloyed with Ti showed better relative elongation, which demonstrates possible reduction of Ti content without losing the strength performance, which naturally occurs when casting transition slabs. To confirm the adequacy of the study, another heat was produced without titanium microalloying. The mechanical properties of such a material do not meet the requirements of EN 10149 and that confirms the impossibility of eliminating the microalloying process of high-strength automotive steel sheets.

Thus, it has been established that steel produced by the developed processes of Ti microalloying is characterized by significantly lower production costs due to smaller content of expensive microalloying elements. At the same time, the complex of mechanical and operational properties remains high, which improves the competitiveness of these products in the market.

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**Toroidal topology and its manipulation in ferroelectric polymers**

**Mengfan Guo**

*Department of Materials Science, University of Cambridge*

*School of Materials Science and Engineering, Tsinghua University*

Topological order in which electrical dipoles rotate quasi-continuously have been widely studied in oxides, and offer the prospect of exotic phenomena and potential applications. I will first introduce the emergence of topological dipolar order in single crystals of ferroelectric polymers, and then their continuous and non-volatile electrical/mechanical manipulations. Various factors create a degenerate landscape for the local polarisation direction, resulting in the static rotation, and enabling dynamic rotations in applied electric fields. Given that polymers absorb infrared radiation in a selective manner, the static and dynamic rotations can be read out using plane-polarised radiation.

**Biography:**

Mengfan Guo is a Royal Society - Newton International Fellow from University of Cambridge. He received his BS and PhD degree from Tsinghua University in 2016 and 2021, respectively. His research interest is ferroelectric materials with an immediate scientific focus and a long-term focus on applications. His main research highlight is the first report of a toroidal topology in a ferroelectric polymer. His papers have been published in Science, Nat. Energy, Nat. Nanotechnol., Nat. Commun., etc.

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### **Addressing Midwakh and E-cigarette use in the Gulf region**

**Sarah Dalibalta**<sup>\*1</sup>, Zinb Makhlouf<sup>2</sup>, Layal Rabah<sup>2</sup>, Fatin Samara<sup>2</sup> and Yehya Elsayed<sup>3</sup>

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A notable decrease in conventional cigarette smoking has been witnessed on a global scale. However, this decrease has been accompanied by an equally striking global increase in the consumption of alternative tobacco products (ATPs), namely e-cigarettes and midwakh in the Arabian Gulf region. Often assumed as healthier alternatives to conventional smoking, we will outline the chemical composition of these two ATPs and their impacts on health. Midwakh contains markedly high levels of tar, nicotine, and various compounds of notable effects on the human body. Similarly, e-cigarettes contain non-negligible amounts of nicotine and other chemical compounds that may not have been extensively investigated. Alarming reports of system specific effects brought about by midwakh and e-cigarette consumption have been reported, although further research is needed to deduce the mechanism. This raises questions around the safety of these two types of ATPs and encourages comprehensive studies globally and regionally.

## **Chitosan- and graphene oxide-based composites for the adsorption of caesium, cobalt and europium from aqueous solution**

**Galina Lujanienė\***

*Center for Physical Sciences and Technology (FTMC), Savanorių Str. 231, LT-02300 Vilnius, Lithuania*

Currently, there is a growing interest in the use of natural, environmentally friendly, cost-effective and biodegradable materials in various fields of science, technology and environmental protection. Fresh, clean water is essential for life on earth, but also for the functioning of many industries. Available wastewater technologies do not provide the required level of purification from persistent pollutants and use harmful synthetic chemicals. It is believed that nanotechnologies and natural materials such as chitosan, natural clays and minerals and adsorbents based on them can improve the efficiency of wastewater treatment technologies. Caesium, cobalt and europium are used in various high-tech applications (e.g. lithium-ion batteries for electric vehicles), while their radioactive isotopes are part of nuclear waste. In addition, europium isotopes are often used as analogues of the toxic trivalent actinides, which have a high migration rate in the environment.

Composites based on chitosan, natural clay of local origin, montmorillonite and zeolite were synthesised using various cross-linking agents (epichlorohydrin, sodium tripolyphosphate, glutaraldehyde) and plasticisers (glycerol)<sup>1</sup>. In addition, composites of magnetic Prussian blue-graphene oxide<sup>2</sup> and chitosan-graphene oxide-maghemite<sup>3</sup> (with Prussian blue crystals of 5-20 nm and particles of magnetite ~10 nm and maghemite < 10 nm) were synthesized. The resulting composites showed high efficiency in the adsorption of Cs<sup>+</sup>, Co<sup>+2</sup>, Eu<sup>3+</sup>, Am<sup>3+</sup> and Pu<sup>4+</sup> from water, including natural river and seawater samples. The experimental data and modelling suggest a complex mechanism controlling the adsorption of Cs<sup>+</sup>, Co<sup>+2</sup> and Eu<sup>3+</sup> ions on the investigated composites. The chitosan-based composites exhibit weak antibacterial properties, which are sufficient to protect the adsorbents from bacterial growth on their surface.

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**Biography:**

Dr. Galina Lujaniene is a senior scientist at the Center for Physical Sciences and Technology (FTMC) in Vilnius, Lithuania. She received her PhD in chemistry from Vilnius University in 1993. Since 1980 she has been working as a senior engineer and a scientist at the Institute of Physics of the Lithuanian Academy of Sciences, which was integrated into the FTMC in 2010, then as a senior scientist and head of the radiochemistry laboratory.

Her research interests include radioanalytical chemistry, environmental radioactivity, and the development of nano-sorbents for the removal of radionuclides and metals from contaminated solutions.

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**Properties of Mesoporous Silicon (MSMPs) as a new adjuvant in the formulation of vaccine complexes**

**Manuel Gómez Del Moral**

*Complutense University, Facultad De Medicina-UCM, Spain*

Vaccinology still presents formidable challenges, not only in infectious diseases such as malaria or AIDS, but also in new cancer treatments, such as immunotherapy. Adjuvants, such as carriers and immunostimulators, are part of new vaccine complexes, and nanotechnology has made its way here. Epitope peptides as well as tumoral antigens are usually very poorly immunogenic and suitable platforms are required with adjuvant capacity to verify immunogenicity and antigenicity of vaccine subunits in vivo. Mesoporous silica and porous silicon particles (MSMPs) possessed intrinsic immunogenicity and can be used as adjuvants [Jiménez-Periáñez A. 2013; Wang, X. et al 2015 and 2016) and carriers. These materials are characterized by being biocompatible, multifunctional, having a high surface area, being easily functionalizable. We have verified in different models (viral and tumor) how MSMPs provide new properties as adjuvants, and could be part of the next new vaccine complexes.

By integrating ancient TCM principles with cutting-edge energy harvesting technology, our research heralds a paradigm shift in healthcare delivery. This convergence not only enhances therapeutic modalities but also fosters a deeper understanding of the synergies between traditional wisdom and modern innovation. Our findings underscore the transformative potential of interdisciplinary collaborations, paving the way for novel solutions that bridge the gap between tradition and progress in healthcare.

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## **Novel potentiometric sensors for continuous metabolite monitoring**

**Idan Tamir\*** & Sharon Lefler

*QuLab Medical Ltd., 71 Hanadiv St., Herzliya Israel*

A novel potentiometric electrochemical sensor has been developed, employing an electrically polarizable working electrode coupled to a field effect transistor (FET). This sensor is designed and built by CMOS fabrication techniques commonly employed in the semiconductor industry. These sensors can continuously monitor redox analytes at the micromolar to millimolar concentration range. We utilized the analyte-specific electrode interaction to tune the specificity of the sensor towards multiple analytes of choice. The resulting potentiometric-tunable electrochemical sensor (PTEchem sensor) is very small (50 X 100 $\mu$ m) and can be fabricated at the tips of chip microprobes fabricated by MEMS techniques. The small size of these microprobes (150 $\mu$ m X 200 $\mu$ m X 1.0-1.5mm) allows the insertion of multiple such sensors into human skin and the continuous and the parallel monitoring of several different metabolites. Dedicated electronics including a wireless transducer facilitate data transfer from this sensor to mobile devices, allowing its use for wearable continuous, multi-metabolite monitoring. The rationale for continuous multi-metabolite monitoring and the clinical use cases will be discussed.

### **Biography:**

Dr. Tamir graduated in Immunology at the Weizmann Institute of Science, followed by a research fellowship at National Jewish Hospital, Denver CO, USA, where he studied B and T cell signaling pathways. After returning to Israel in 2000, Dr. Tamir was the CEO of life-sciences accelerator, co-founding over 20 companies that have collectively raised over \$100M with three notable exits. Dr. Tamir then joined a US-based Venture Capital group based in Richmond VA that brought Israeli medical device companies and products to the North American market. Since 2017, Dr. Tamir has been the co-founder and CEO of QuLab Medical.

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**Rashba metasurfaces – strain-tuned surface states towards perfect darkness**

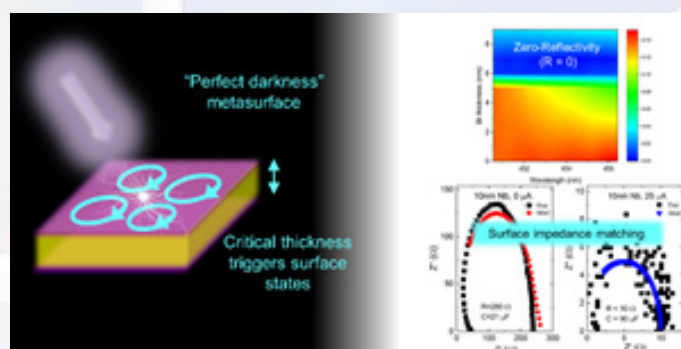
Anna Kusmartseva<sup>1\*</sup>, Binglei Zhang<sup>2</sup>, Yang Liu<sup>2</sup>, Yi Luo<sup>2</sup>, James Vincent-Ward<sup>1</sup>, Fatemah Alkallas<sup>3</sup>, Amira Ben Gouider Trabelsi<sup>3</sup> and Fedor Kusmartsev<sup>4</sup>

<sup>1</sup> Department of Physics, Loughborough University, Loughborough LE11 3TU, UK

<sup>2</sup> Microsystem and Terahertz Research Center, Chengdu, 610200, P.R. China

<sup>3</sup> Department of Physics, College of Science, Princess Nourah bint Abdulrahman University, Riyadh 11671, Saudi Arabia

<sup>4</sup> College of Art and Science University, Abu Dhabi, UAE



Metallic films are well-known for their high reflecting properties and are often utilized as mirrors in technological applications such as radars, telescopes and mobile communications. In the present work we will demonstrate how by reducing the dimensionality of nanometer thick metal films from 3D to 2D we can obtain a perfectly dark antireflective metasurfaces. This phenomenon of perfectly dark zero reflectivity has been successfully observed across various metals, including Sn, Ag, Au, Pt, Bi, and Nb, showcasing its broad applicability.<sup>1</sup>

The underlying principle lies in the emergence of surface states (SfS), where the Rashba effect is strong, giving rise to the formation of Rashba metamaterial and metasurface (RMM) structures. Remarkably, these RMMs can be fine-tuned to act as high-resolution Veselago lenses and have been shown to sustain highly mobile 2D electron gas (2DEG). Any metal nano-films can be transformed into Rashba metasurfaces capable of sustaining regions of perfect darkness for all incident light at all incident angles. This pioneering discovery will shift the paradigm in developing lossless light applications based on any combination of dielectric substrate and the RMMs - ranging from solar energy harvesting to high-precision sensors for medical diagnostics and THz communications.

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**Biography:**

Dr Anna Kusmartseva has an established track record in high-pressure condensed matter physics, and strain-effect in low-dimensional systems. Her vision is to promote topological materials, exploring and harnessing their potential in applications related to renewable energies and quantum technologies. Dr Kusmartseva has lead many interdisciplinary projects and received funding from multiple European (e.g. Alexander von Humboldt foundation) and UK funding bodies (e.g. EPSRC and the Royal Society). She currently holds the internation collaboration award with Princess Nourah bint Abdulrahman University in Saudi Arabia and actively strives to strengthen the presence of under-represented communities in STEM disciplines.

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## **Preliminary Study of Wound Oxygenation Comparing Skin Substitutes and Dressings**

Aubrey Woodrood PhD, Joshua Moote, Jim Polansky MS, **Linwood R Haith MD**, William Hickerson MD

**Background:** Improving oxygen delivery to challenging wound types has been shown to optimize and accelerate several key contributors to healing. This study aims to compare selective skin substitutes and primary dressings PermeaDerm™, INTEGRA™ Bilayer Matrix Wound Dressing (non-meshed), and NovoSorb® BTM's ability to transfer oxygen to the wound.

**Methods:** Visual and quantitative methods were employed to measure gas and fluid movement across selective skin substitutes.

**Results:** Fluids do not move across solid silicone membranes or urethane foam. Oxygen moves across solid silicone membrane inversely proportional to the thickness of the membrane. Oxygen moves across PermeaDerm 5.63 times faster than across INTEGRA™ Bilayer Matrix Wound Dressing and 2.0 times faster than NovoSorb® BTM.

**Conclusions:** PermeaDerm™ functions like a membrane oxygenator, potentially augmenting atmospheric oxygen delivery to healing wounds.

### **Biography:**

Linwood R. Haith, Jr, MD is Academic Chair and Clinical Professor Department of Surgery, Drexel University College of Medicine. He was President of the American Burn Association (ABA) 2018 and remains active on the Verification Committee and Chair of the Fellow of American Association Committee. He has been strongly involved in clinical research on burn patients and has published 60 journal articles and a chapter, "Burns/ Inhalation," in *The Trauma Manual* 2nd Edition. He has also presented locally, nationally, and internationally on a range of topics related to the care of burn patients.

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**Synthesis and Characterization of  $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$  and  $\text{La}_2\text{NiTiO}_6$  Double Perovskite Nanoparticles**

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In the present work,  $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$  and  $\text{La}_2\text{NiTiO}_6$  nanoparticles were synthesized by the modified Pechini method.  $\text{LaNi}_{0.5}\text{Ti}_{0.5}\text{O}_3$  was calcined at 1073 K for 17 h or 100 h, while  $\text{La}_2\text{NiTiO}_6$  was calcined at 1273 K for 135 h. The materials were characterized by X-ray fluorescence, X-ray diffraction coupled to the Rietveld method, scanning electron microscopy, and magnetic measurements. X-ray fluorescence was carried out using a Rigaku Primini spectrometer equipped with a Pd X-ray tube operating at 50 W (40 kV, 1.25 mA). X-ray diffraction measurements were performed in a Rigaku Miniflex II X-ray diffractometer equipped with a graphite monochromator, using  $\text{CuK}\alpha$  radiation (30 kV and 15 mA). Micrographs were obtained from a scanning electron microscope (SEM, Model Quanta™ 450 FEG, FEI Company, Hillsboro, OR, USA) operating with an accelerating voltage of 20 kV. DC magnetic measurements as a function of temperature, in the zero-field-cooled process, applying a magnetic field of 100 Oe, were performed using an MPMS 3 SQUID magnetometer and a Cryogenic SX-600 SQUID magnetometer. The double perovskite calcined at 1073 K for 17 h presented orthorhombic symmetry with  $Pbnm$  space group, glazer notation  $a-a-c^+$ , mean particle size of  $31.9 \pm 1$  nm, random ordering of  $\text{Ni}^{2+}$  and  $\text{Ti}^{4+}$  cations, Néel temperature close to 15 K, and magnetic moment of  $1.29 \mu_B$ . By increasing the calcination time, this material showed the same symmetry, space group and glazer notation, a mean particle size of  $50.7 \pm 2$  nm, short-range ordering of  $\text{Ni}^{2+}$  and  $\text{Ti}^{4+}$  cations, Néel temperature around 12 K, and magnetic moment of  $0.96 \mu_B$ .  $\text{La}_2\text{NiTiO}_6$  presented a monoclinic crystal structure, with  $P2_{1/n}$  space group, glazer notation  $a-a-c^+$ , mean particle size of  $80.0 \pm 5$  nm, rock salt ordering of  $\text{Ni}^{2+}$  and  $\text{Ti}^{4+}$ , Néel temperature of approximately 23 K, and magnetic moment of  $2.75 \mu_B$ .

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**Biography:**

Pablo V. Tuza is Chemical Engineering from Universidad Técnica Particular de Loja, Ecuador. Also, he achieved his M.S. & Ph.D. from the Tecnologia de Processos Quimicos e Bioquimicos Program at Universidade Federal do Rio de Janeiro, Brazil. He acts on the following subjects: Nanomaterials, Heterogeneous Catalyst, Petrochemical precursors and processes. Recently, he was invited as a reviewer for the Powder Diffraction Journal due to his works on Double Perovskite materials containing La, Ni, Ti, and Co. He works as an Occasional Professor at the Facultad de Ciencia e Ingeniería en Alimentos y Biotecnología from the Universidad Técnica de Ambato, Ecuador.



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**Utilize pMAIRS to Evaluate the Conformation and Orientation of of  $\alpha$ -Synuclein(61-95) in Monolayer at Interface with Residue Level Resolution**

**Chengshan Wang**

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Membrane proteins cause challenges for the major techniques (i.e., X-ray crystallography, NMR, and cryo-Electron Microscopy) to determine protein's structure with high resolution. For example, it is difficult for membrane proteins to form single crystal structure required by X-ray. For NMR, the tumbling rate will be decreased substantially for membrane proteins. As a recent developed technique, cryo-Electron Microscopy (cryo-EM) requires mono-dispersed and unified samples in frozen state. Therefore, equilibrating conformations in some residues in protein's structure are not welcome. In addition, all the techniques above cannot provide high resolution results for monolayer structure, which is the native state of membrane proteins. To address this issue, surface FT-IR techniques were developed and p-polarized Multiple Angle Incidence Resolution Spectroscopy (pMAIRS) was recently developed with the capability to quantitatively determine the tilt angle of a vibration even in monolayer at interface. Here, the nonamyloid component (NAC), which spans residues 61–95 of  $\alpha$ -synuclein, was studied here because it interacts with the amphiphilic membrane structure and directly relates with both Parkinson's disease and Alzheimer's disease. The overall tilted angle of the axis of NAC was evaluated to be  $30.1^\circ$  by pMAIRS. A  $^{13}\text{C}$  isotopic label was introduced into the backbone carbonyl at the position of 93G in NAC. The  $^{13}\text{C}$  isotopic labeled carbonyl generated a new  $^{13}\text{C}$  amide I band, which was then analyzed by pMAIRS to reveal the tilt angle of the axis at 93G to be  $\sim 0^\circ$ . This means that the axis at 93 G is parallel to the interface. Other positions around N-terminal residues (e.g., 68G) is more perpendicular in freshly prepared monolayer. After compressed for several hours, 68G was found to equilibrate with two conformations. In general, pMAIRS can evaluate conformation and orientation of NAC in residue level even in monolayer to supplement other major techniques.

**Biography:**

Dr. Chengshan Wang is a biophysical chemist and received his doctoral degree from University of Miami (U.S.A.) for a work on surface spectroscopy of proteins in 2008. During his postdoc phase, he extended his research to Parkinson's disease. In 2011 he started his career as a faculty member in Chemistry Department of Middle Tennessee State University. He was promoted to Associate Professor in July, 2017.

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**Effect of polarization on Nb and Mn doped BaTiO<sub>3</sub> ferroelectric on its photovoltaic, electrical and electrical properties.**

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In this work, the effect of the polarization of ferroelectric BaTiO<sub>3</sub> films doped with Mn and Nb is experimentally studied, in a capacitor configuration formed by a heterostructure using ZnO/Al and CuO for the photovoltaic cell. The materials were synthesized with the sol-gel method, which consists of the stoichiometric mixture of each of the precursors. The synthesis of ZnO doped with Al was obtained through the sol-gel process, generating nanoparticles that grouped together to form a solid target that were deposited by RF sputtering. For the synthesis of BaTiO<sub>3</sub>, the precursors used were titanium butoxide and barium acetate to obtain a stable solution. In the case of the synthesis of the CuO solution, it was carried out using the reagents of copper acetate, glycerol, triethylamine and methanol as a solvent. For these last 2 solutions, the deposition of thin films was carried out using the spin-coating technique. The physicochemical properties of the materials were analyzed using: SEM, XRD, UV-Vis, I-V curves and ferroelectric hysteresis loops. The results of the CuO solution on the ZnO surface were analyzed by SEM images and demonstrated that the solution can be dispersed on the surface without problems. The bandgap energy corresponding to CuO is approximately 2 eV. The x-ray diffractograms show the crystalline phase corresponding to BaTiO<sub>3</sub> including changes due to doping. At this point, doping allows the band gap of BaTiO<sub>3</sub> to be reduced, allowing a greater use of solar radiation in the separation of the photo-carriers where their photo-response will be evaluated. In the results obtained in the I-V measurements, it is observed that the photo-response of the complete system is favorable since the photovoltaic effect increases; depending on the induced polarization, it is possible to control the ferroelectric properties to a greater extent<sup>1-2</sup>

1. ACS Energy Lett. 2018, 3, 5, 1176–1182

2. Nature Nanotechnology, 2010, 5, 143–147

**Biography:**

Dr. Jesús Iván Peña Flores completed his bachelor's degree in chemical engineering, master's degree and doctorate in materials science at the Benemérita Universidad Autónoma de Puebla (BUAP). During the degree, the selected topic was about photocatalysis using copper-doped TiO<sub>2</sub> for the degradation of organic compounds. In the case of the master's and doctorate, the topics were about the synthesis of thin films using chemical methods such as sol-gel, particle synthesis and wettability properties. Currently, the proposed research is about the ferroelectric properties of BaTiO<sub>3</sub> doped with Mn-Nb to reduce its bandgap using an arrangement of oxides for photovoltaic cells.

# Day-2 Virtual

## Microscopic behavior of self-diffusion in liquid Sn and Pb using molecular dynamics simulation

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Self-diffusion in liquid metal is essential property to understanding dynamics of atoms. For analysis of the dynamics in liquid metals, molecular dynamics (MD) simulation is powerful tool to evaluate the self-diffusion combined with the liquid structure. Especially, liquid Sn has been reported for unique liquid structures characterized by a shoulder which represents a hump on the high wave vector side of the first peak of structure factor<sup>[1]</sup>. This study aimed to clarify the effect of a unique liquid structure with a shoulder in liquid Sn on the self-diffusion in comparison of liquid Pb which is the representative element that reproduces a hard-sphere model through MD simulation.

MD simulation was conducted using LAMMPS package (version: 19 Sep 2019). A total of 4096 atoms of Sn and 4000 atoms of Pb arranged in a cubic simulation box with standard periodic boundary conditions have been considered, respectively. The targeted calculation was running during 100 ps using the NVT ensemble and then time series data of atomic positions were obtained at 573 K in liquid Sn and at 773 K in liquid Pb, respectively.

The mean-square diffusion depths were calculated from the time series data of all position and self-diffusion coefficient of Sn and Pb, respectively. The values of self-diffusion coefficients of Sn and Pb at 100 ps were  $2.29 \times 10^{-9} \text{ m}^2\text{s}^{-1}$  and  $2.56 \times 10^{-9} \text{ m}^2\text{s}^{-1}$  that were in good agreement with the reference data under the microgravity condition<sup>[2,3]</sup>. From the local atomic configurations and time series analyses of individual atoms, the microscopic behavior of liquid Sn is unlike that of liquid Pb because the atomic motions of Sn are inhibited by the atoms around the next nearest neighbor sites in the range that corresponds to the shoulder appearing in the pair distribution function of liquid Sn as well as in the structure factor of liquid Sn.

[1] T. Itami, S. Munejiri, T. Masaki, H. Aoki, Y. Ishii, T. Kamiyama, Y. Senda, F. Shimoji, and K. Hoshino: Phys. Rev. B, 2003, vol. 67, 064201. [2] Y. Malmejac and G. Frohberg: in Fluid Sciences and Materials Science in Space: A European Perspective, H.U. Walter, ed., Springer Berlin Heidelberg, Berlin, Heidelberg, 1987, pp. 159–190. [3] G. Mathiak, A. Griesche, K.-H. Kraatz, and G. Frohberg: J. Non Cryst. Solids, 1996, vol. 205–207, pp. 412–416

### Biography:

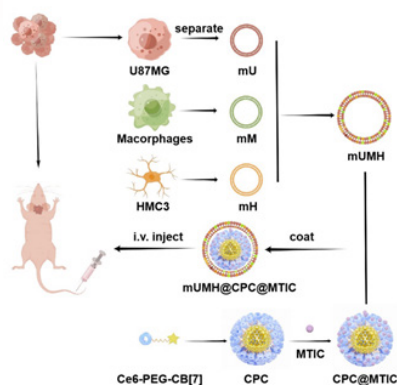
**Masato Shiinoki** is an assistant professor (without tenure) of Applied Mechanics and Aerospace Engineering at Waseda University, Japan. He has completed his Doctor of Engineering from Waseda University. His work focuses specifically on the elucidation of diffusion mechanisms in liquid metals through a combination of diffusion measurement and MD simulation. He received a Research Encouragement Award to study about accuracy measurements of diffusion coefficients in liquid metals based on microgravity data from the Japan Society of Microgravity Application in 2021. His presentation discusses how liquid structures affect the dynamics represented by diffusion behavior using MD simulation.

## Tumor microenvironment targeting for glioblastoma multiforme treatment via hybrid cell membrane coating supramolecular micelles

Xiaobei Huang

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Glioblastoma multiforme (GBM) is one of the most common primary intracranial tumors in the central nervous system with poor prognosis, high invasiveness, risk of recurrence and low survival rate. Thus, it is urgent and vital to develop drug effective delivery systems that efficiently to traverse the blood–brain barrier and targeted transport therapeutic agents into the GBM tumor site for the treatment of brain tumors. Recently, amphiphilic cucurbit[7]uril-polyethylene glycol-hydrophobic Chlorin e6 (CB[7]-PEG-Ce6) polymer was designed, prepared, and self-assembled into micells (CPC) in an aqueous solution, and chemo drug methyl-triazeno-imidazole-carboxamide (MTIC), loaded into the cavity of CB[7] was subsequently coated with hybrid membrane mUMH (HMC3 membrane: macrophages membrane: U87MG membrane = 1:1:2) to afford mUMH@CPC@MTIC. The surface hybrid membrane mUMH potential to enhance the targeted delivery of CPC@MTIC to GBM tissue. Bioactive MTIC was released from the cavity of CB[7] in response to the high spermine level in GBM tumor microenvironments for effective tumor chemotherapy. The biomimetic mUMH@CPC@MTIC exhibited superior antitumor efficacy against GBM in mice. These findings provide new strategies for the design of biomimetic nanoparticle-based drug delivery systems and promising therapy of GBM.



Xiaobei Huang

Associate Research fellow

Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Science.

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## CO<sub>2</sub> permeation on Zn<sup>2+</sup> modified Al<sub>2</sub>O<sub>3</sub>-carbonate membranes

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<sup>2</sup> Department of Materials Science and Engineering, Northeastern University

<sup>3</sup> School of Engineering, Newcastle University

Dual phase ceramic/molten carbonate membranes have received increased attention for CO<sub>2</sub> separation application due to the benefits related to cost, high temperature stability as well as environmental impact as opposed to traditional processes. It has been shown that modifying the composition of the molten salt phase allows for tuning the conductivity and CO<sub>2</sub> permeability, opening new dimensions to membrane design. In this work, in an attempt to tune the molten carbonate composition, a ZnAl<sub>2</sub>O<sub>4</sub> layer was deposited at the interface on a Al<sub>2</sub>O<sub>3</sub>/molten carbonate membrane. It was found that a LiAlO<sub>2</sub> interface layer was formed with the dissolution of ZnO into the molten carbonates phase and enhanced the CO<sub>2</sub> permeability of such ZnAl<sub>2</sub>O<sub>4</sub>/Al<sub>2</sub>O<sub>3</sub>/carbonate membrane, in comparison with the pristine Al<sub>2</sub>O<sub>3</sub>/carbonate membrane. This enhancement was found to be due to the dissolved ZnO species in the molten salt phase which increased the membrane conductivity. On the other hand, the increase in Zn<sup>2+</sup> concentration led to a decrease in CO<sub>2</sub> permeability.

### Biography:

Liu Qu, obtained PhD from University College London, MSc from Imperial College London and BEng from University of Science and Technology Beijing. She is appointed as Lecturer at Shenyang Ligong University. Her research interests include materials design for gas separation membranes and heterogeneous catalysts.

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**Effects Of Dietary Solvents on Microhardness and Inorganic Elemental Composition of Computer-Assisted Design/Computer-Assisted Manufacturing Dental Composites.**

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<sup>2</sup> Biomaterials Research Laboratory, Faculty of Dentistry, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

The exposure of dental composites to food and beverages in the oral cavity is inevitable. Based on Food and Drug Administration (FDA) guidelines, dietary solvents can be used to mimic food and beverages. Recent years showcased the use of nanotechnology to improve the physical properties of dental composites. In addition, industrial polymerization processes involving high temperature and/or high pressure has been implemented to produce computer-assisted design/computer-assisted manufacturing (CAD/CAM) dental composites. Objective of this study was to evaluate the effect of dietary solvents on microhardness and inorganic elemental composition of CAD/CAM dental composites. 50 specimens with dimensions 12mm x 14mm x 1.5mm were prepared for direct composite (Filtek Z350 XT [FZ]), indirect composite (Shofu Ceramage [CM]), and three CAD/CAM composites (Lava Ultimate [LU], Cerasmart [CS], and Vita Enamic [VE]). The specimens were randomly divided into 5 groups (n=10), conditioned for 1-week at 37°C: air (control), distilled water, 0.02 N citric acid, 0.02 N lactic acid and 50% ethanol-water solution. The specimens were subjected to microhardness test (KHN) using Knoop hardness indenter. Air (control) and representative postconditioning specimens with the lowest mean KHN value for each material were analyzed using energy dispersive X-ray spectroscopy (EDX). Statistical analysis was done using one-way ANOVA and post hoc Bonferroni test at a significance level of  $p = 0.05$ . Mean KHN values ranged from  $39.7 \pm 2.7$  kg/mm<sup>2</sup> for FZ conditioned in 50% ethanol-water solution to  $79.2 \pm 3.4$  kg/mm<sup>2</sup> for VE conditioned in air. With exception to LU, significant differences were observed between materials and dietary solvents for other composites investigated. EDX showed stable peaks of the inorganic elements between air (control) and representative postconditioning specimens. The microhardness of dental composites was significantly affected by dietary solvents, except for one CAD/CAM composite [LU] with no changes in the inorganic elemental composition of CAD/CAM dental composites.



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**Biography:**

Dr. Selva Malar Munusamy is a Prosthodontist at the Department of Restorative Dentistry, Faculty of Dentistry, Universiti Malaya, Kuala Lumpur, Malaysia. She received her BDS from Universiti Malaya in 2007 and Clinical Masters (Prosthodontics) from The University of Manchester, UK in 2015. She is a member of the Royal College of Surgeons of Edinburgh, UK. Her achievements include best oral presenter in Malaysia International Dental Exhibition and Conference 2019, gold award in International Invention and Innovation in Dentistry Exhibition (IIIDENTEX) 2022 & 2023 and National Record for the First Oral Health Braille Book in The Malaysia Book of Records 2023.

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**Mechanical stability of carbon/ramie fiber hybrid composites under hygrothermal aging**

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<sup>1</sup> School of Air Transportation, Shanghai University of Engineering Science, Shanghai 201620, China

Hybrid composites containing carbon fibers and ramie fibers in an epoxy polymer matrix were prepared (denoted as CRFRP), after which the composites were immersed in distilled water at three different temperatures (20, 40, and 60 °C) for a period up to 2 months. Water absorption tests and static (tensile and flexural) and dynamic (low-velocity impact) mechanical tests were then conducted on the hygrothermally-treated composites to explore their hydrothermal aging mechanism. Results show that water uptake by CRFRP composites was enhanced by increasing the hygrothermal treatment temperature or aging time, with the water uptake obeying a Fickian diffusion model. Hygrothermal aging decreased the tensile strength, tensile modulus, flexural strength and flexural modulus of the CRFRP composites, though enhanced the impact absorption energy since the ramie fibers had greater plasticity and deformability after aging. Based on the experimental findings, a plausible mechanism was developed for the hydrothermal aging of the hybrid composites. Importantly, CRFRP composites were lighter than carbon fiber-reinforced composites (CFRP), whilst offering similar all-round performance, suggesting CRFRP composites may be useful in applications where CFRP composites have traditionally been used.

**Biography:**

CAI Ming : Shanghai University of Engineering Science, Lecture  
NANYANG TECHNOLOGICAL UNIVERSITY, Visiting Scholar.

## Approaches to the design of efficient and stable catalysts for biofuel reforming into syngas: Doping the mesoporous $\text{MgAl}_2\text{O}_4$ support with transition metal cations

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<sup>1</sup>Federal Research Center Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

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The mesoporous  $\text{MgAl}_2\text{O}_4$  support is promising for the design of efficient and stable to coking catalysts for natural gas and biofuel reforming into syngas. This work aims at doping this support with transition metal cations (Fe, Cr, Ti) to prevent the incorporation of Ni and rare-earth cations (Pr, Ce, Zr), loaded by impregnation, into its lattice along with providing additional sites for  $\text{CO}_2$  activation required to prevent coking. Doped  $\text{MgAl}_{1.9}\text{Me}_{0.1}\text{O}_4$  (Me = Fe, Ti, Cr) mesoporous supports prepared by the one-pot evaporation-induced self-assembly method were single-phase spinels. Nanocomposite active component  $\text{Pr}_{0.3}\text{Ce}_{0.35}\text{Zr}_{0.35}\text{O}_2 + \text{NiRu}$  was deposited by impregnation.  $\text{Pr}_{0.3}\text{Ce}_{0.35}\text{Zr}_{0.35}\text{O}_2$  preserves its structure after calcination including sintering by e-beam irradiation,  $\text{MgAl}_2\text{O}_4$  remains mesoporous, and NiO, and  $\text{RuO}_2$  phases are identified. In methane dry reforming, the positive effect of  $\text{MgAl}_2\text{O}_4$  support doping was observed in a higher turn-over frequency as well as the highest efficient first-order rate constant for the Cr-doped catalyst. In the reaction of ethanol steam reforming, the efficiency of catalysts on the doped supports is comparable, while exceeding that of Ni-containing supported catalysts reported in the literature. Coking stability was provided by a high oxygen mobility in the surface layers estimated by the oxygen isotope heteroexchange with  $\text{C}^{18}\text{O}_2$ . A high efficiency and coking stability were demonstrated in the reactions of methane dry reforming and ethanol dry and steam reforming in concentrated feeds for the structured catalysts with a nanocomposite active component on the Fe-doped  $\text{MgAl}_2\text{O}_4$  support loaded on the FeCrAl-alloy foil or plate substrates. Using e-beam sintering of supported layers allows to decrease processing temperature, reduce internal thermal stresses and increase nanocomposite active component dispersion and metal-support interaction, thus helping to increase activity and coking/thermal shock stability.

Different parts of this work are carried out within BIC SB RAS FWUR-2024-0033 budget project and Russian Science Foundation Project 23-73-00045.

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**Biography:**

Professor Vladislav Sadykov is the chief scientist at the Boreskov Institute of Catalysis and Professor of Novosibirsk State University. His current research interest includes heterogeneous catalysis of red-ox processes for the energy production, catalytic processes of hydrogen and syngas generation, membrane reactors, technologies of nanophase and nanocomposite materials synthesis, solid state ionics. He has published more than 500 papers in peer-reviewed journals, four monographs and 7 Chapters in books. He is the member of the Editorial Boards of Applied Catalysis A, Membranes and Energies (MDPI), the member of the Materials Research Society (USA) and Russian Mendeleev Chemical Society.

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**Spectroscopic ellipsometry and B-spline coefficients of non-hydrogenated amorphous silicon for amorphous silicon based semiconductors**

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<sup>1</sup>Department of Physics and Astronomy, College of Science, King Saud University, P.O. Box 2455, Saudi Arabia

<sup>2</sup>Department of Physics and Astronomy, College of Science, Ohio University, Athens, Ohio 45701, United States

<sup>3</sup>School of Electrical Engineering and Computer Science, Ohio University, Athens OH 45701, United States

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Amorphous silicon has been playing a crucial role in renewable energy and energy storage devices. Here, we report on the application of Kramers–Kronig (KK) consistent B-spline parametric model to the complex dielectric function of non-hydrogenated amorphous silicon (a-Si). a-Si thin films were deposited onto quartz and thermal-SiO<sub>2/c</sub>-Si(100) substrates using radio frequency magnetron sputtering at a relatively low temperature of 195 K (−78°C). Room temperature ex-situ spectroscopic ellipsometry (SE) was employed post-growth with high resolution, and the energy-slicing B-spline parametric model was implemented within a multilayered structure using fourteen non-vanishing B-spline series expansion coefficients {c<sub>i</sub>}, which resulted in accurate determination of the complex dielectric function, optical bandgap, and film thickness simultaneously. The fitting parameter correlation matrix was further obtained and analyzed in detail. The obtained B-spline parameterization represents an accurate basis reference for a-Si over the wide UV-VIS-NIR spectral range 270 - 1240 nm corresponding to 1.0 - 4.6 eV, and it was applied accurately to two amorphous silicon based semiconductors until accurate fittings were attained, which are the non-hydrogenated phase a-Si deposited under different growth conditions and the hydrogenated phase a-Si<sub>x</sub>H<sub>1-x</sub> with various alloyed hydrogen at. %.

**Biography:**

Dr. Mohammad Ebdah is an assistant professor at King Saud University and a fellow of Ohio University, who is specialized in spectroscopic ellipsometry. Such a model based experimental technique known for its accuracy to explore the optical properties of crystalline and amorphous semiconductors. He also uses other techniques such as reflectometry, diffused reflectance, and photoluminescence to unveil the dielectric and optical functions of semiconductors. Recently, he developed with colleagues a series expansion optical model for amorphous semiconductors, and he has ongoing equation that is under development for amorphous semiconductors.

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**Specific and label-free biosensing with a novel biologically-modified field-effect transistor (BioFET)**

**Gil Shalev**<sup>1,9\*</sup>, Soumadri Samanta<sup>1</sup>, Vinay S. Tiwari<sup>2</sup>, Sumesh Sadhujan<sup>3</sup>, Sherina Harilal<sup>3</sup>, Avital Eisenberg-Lerner<sup>5</sup>, Ziv Rotfogel<sup>5,6</sup>, Evgeny Pikhay<sup>4</sup>, Ruth Shima-Edelstein<sup>4</sup>, Doron Greental<sup>4</sup>, Muhammad Y. Bashouti<sup>3,9</sup>, Barak Akabayov<sup>2</sup>, Izhar Ron<sup>1</sup>, Yakov Roizin<sup>4</sup>, Offer Erez<sup>7,8</sup>

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<sup>2</sup> Department of Chemistry and Data Science Research Center, Ben-Gurion University of the Negev, 8410501, Beer-Sheva, Israel

<sup>3</sup> Department of Solar Energy and Environmental Physics, Swiss Institute for Dryland Environmental and Energy Research, J. Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Midreshet Ben-Gurion 8499000, Israel

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Transistor-based sensing is the holy grail of medical diagnostics as it supports low-cost self-use and point-of-care tests in a multiplexed manner from ultra-small physiological samples. We recently developed the Meta-Nano-Channel (MNC) field-effect biosensor for specific and label-free sensing of antigen-antibody interactions. The novelty of the MNC biosensor is twofold: 1) it allows to optimize the coupling between the electrostatics of the biological interactions and the nanometric readout current, and 2) it allows to electrostatically affect the biological complexes and shape the interaction. These attributes yield an optimized and tunable sensing performance. The MNC biosensor is fabricated in a high-volume silicon chip factory for this research, which implies excellent electronic performance in terms of gain and noise coupled with excellent repeatability, stability and robustness. In the current talk I will present specific and label-free sensing of various target molecules in 0.5  $\mu$ L drops of 1:100 diluted serum/plasma with a limit-of-detection (LOD) in the range of 1 fg/ml, dynamic range extending to 10 orders of magnitude and with excellent linearity and sensitivity. Importantly, the attributes of the MNC biosensor allow for a tunable sensitivity and a tunable dynamic range. We believe the new paradigm introduced by the MNC biosensor shapes the path for future medical diagnostics.

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## **Self-Healing Silsesquioxane-Based Materials**

**Anna Kowalewska**

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Polymeric self-healing materials (SHM) are of growing interest due to the dynamic properties that can improve their performance and extend their service life. SHM can self-regenerate after a crack or external mechanical damage, spontaneously or after stimulation by environmental conditions. These beneficial aspects help reduce the amount of synthetic materials in the environment, which is in line with the 4Rs of the circular economy (reduce, reuse, recycle and recover).

Polyhedral oligosilsesquioxanes (POSS) are the smallest known hybrid silica nanoparticles with a well-defined structure. Their key features stem from their unique hybrid morphology with a nanoscale inorganic core of uniform size composed of silicon and oxygen atoms and surrounded by eight functional groups. POSS have gained great interest over the past two decades due to the fact that they can be functionalized quite easily to produce materials with variable structure and properties.

The presence of appropriate functional groups on the silica core allows the formation of dynamic bonds with POSS molecules and makes them an active component of SHM, both as crosslinking agents and factors that can influence dynamics of macromolecules in the polymer matrix required for effective self-healing. It can be achieved by reversibly releasing bulky POSS cages through Diels-Alder reactions, metal-ligand interactions or thiol/disulfide chemistry. Another strategy is based on the formation of separate inclusions in the polymer matrix through hydrophobic interactions and POSS aggregation, which can be achieved by reversible release of POSS or formation of separate inclusions in the polymer matrix through hydrophobic interactions and POSS aggregation. The specific chemistry and interactions occurring in self-repairing POSS-based systems makes them interesting and versatile next-generation materials with improved mechanical properties, suitable for various applications (e.g., repairable coatings, sealants, sensors, soft materials for tissue engineering, drug delivery and wound healing).



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**Biography:**

Prof. Anna Kowalewska received her PhD (Synthesis and reactivity of sterically hindered silanes, 1998) and postdoctoral (*Application of sterically hindered carbosilanes in polymer chemistry*, 2010) degrees in chemistry from Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences in Lodz (Poland). She was awarded the title of professor of chemical sciences in 2022. Her research work in the field of organosilicon chemistry is documented by more than 70 scientific publications and patents. Her current research interests include organosilicon polymers with complex morphology; ladder- structured polysilsesquioxanes and their polyhedral analogs; synthesis, physicochemical properties and applications of hybrid materials; organosilicon polymers with antimicrobial properties; well-defined nanostructured materials and surface science.

**The dominance of pretransitional effects in liquid crystal based nanocolloids: MBBA with transverse and 5CB with the longitudinal permanent dipole moment plus BaTiO<sub>3</sub> nanoparticles**

Aleksandra Drozd-Rzoska and **Sylwester J Rzoska**

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The impact of isotropic liquid – nematic and nematic – solid crystal phase transitions is tested via wide temperature range and pressure high-resolution broadband dielectric spectroscopy, covering the low-frequency (LF), static, and dynamic domains. Studies were carried out in MBBA (4-methoxybenzylidene-4'-butylaniline) with the transverse location of the permanent dipole moment and 5CB (pentyl-cyano-biphenyl) with the longitudinal location of the permanent dipole moment plus BaTiO<sub>3</sub> paraelectric nanoparticles.

The distortions-sensitive analysis shows the strong and long-range dominance of pretransitional effect for both sides of the isotropic liquid – nematic weakly discontinuous transition. The unique evidence from the pretransitional impacts has also been evidenced for the surrounding of the strongly discontinuous nematic – solid transition, particularly for the solid crystal phase. It follows the critical-like patterns despite the inherently discontinuous nature of the transition. The phenomenon can be explained by linking the Lipovsky model to the Mossotti catastrophe concept under quasi-negative pressure conditions. The explicit preference for the 'critical-like' evolution of the apparent activation enthalpy is worth stressing for dynamics. Finally, the dissipation factor's long-range, 'critical-like' behavior ( $D = tg\delta$ ), covering the isotropic liquid and nematic phases, is shown. The results presented show the significant impact of the permanent dipole location and the concentration of nanoparticles, which can lead to the permanent endogenic orientation of LC molecules, and for a selected concentration and pressure tuning, a continuous isotropic – nematic transition can appear.

This research presented research was supported by the National Center for Science (NCN, Poland), grant number NCN OPUS 2022/45/B/ST5/04005, headed by S. J. Rzoska.

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**Biography:**

available at ORCID: 0000-0002-2736-2891 and 0000-0001-8510-2388.  
See also the X-PressMatter lab page: <https://young4softmatter.pl>

## Polycatenanes Formed of Self-Assembled Metal Organic Cages

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In this contribution, of properties of poly-[n]-catenanes composed of interlocked M12L8 icosahedral nanometric cages are investigated by Quantum Chemical (QC) calculations and X-ray diffraction experiments [1]. The TPB (exotridentate trispyridyl benzene) ligand and ZnCl<sub>2</sub>, in the presence of appropriate templating molecules (Figure 1), form metal-organic nanocages microcrystalline materials. Single-crystal X-ray data collected at 100 K allowed to solve the structure and to detect guest molecules at the internal walls together with highly disordered solvent in the central part. The processes of guests absorption and release are driven by intramolecular and intermolecular interactions. QC calculations [2] were used to study packing energies and host-guest interactions. Key factors in the formation of the poly-[n]-catenane and in solvent exchange are rationalized through a mechanism of "closed-open" dynamic channels. The labile nature of the Zn-N coordination bonds allows the recyclability of TPB ligand in water, thus making these materials very good candidates in green chemistry applications.

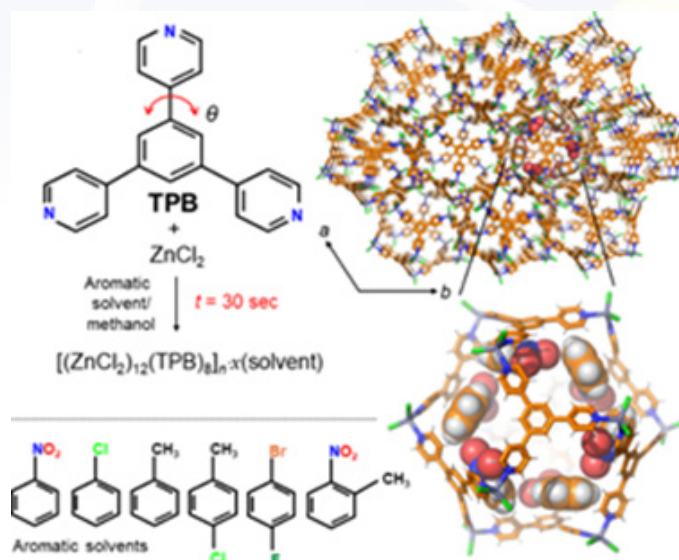


Figure 1. Sketch of the synthesis of poly-[n]-catenane and a view of the crystalline phase.

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**Unique features of mRNA-LNP Covid-19 vaccine nanoparticles explaining the acute adverse effects and post-vaccine syndrome**

**Janos Szebeni**

*Nanomedicine Research and Education Center, Department of Translational Medicine, Semmelweis University & SeroScience LCC, Budapest, Hungary*

The success of Pfizer-BioNTech's Comirnaty and Moderna's Spikevax mRNA vaccines in attenuating the symptoms of Covid-19 is due, among others, to some unique features of mRNA-carrier lipid nanoparticles (mRNA-LNPs). These include the use of ionizable and PEGylated lipids in the NPs, chemically modified spike-protein (SP) mRNA as antigen code, and the capability of these LNPs to induce robust humoral and cellular immune response. This new gene therapy platform promises treatments for many incurable diseases. As a less commended benefit of these vaccines for the future is that vaccination of billions all over the world expanded the horizon of immune toxicology by bringing to surface a new disease; postvaccination syndrome (PVS). Importantly, the occasionally severe long-term symptoms of PVS are also typical of Covid-19 and long Covid, as the SP is a common pathogenic factor in these conditions. PVS is a subject of intense scientific and public debates, thus, understanding the extent of problem and its scientific background is essential. Accordingly, the presentation will update the prevalence and incidence of different PVS symptoms and detail some in vitro and in vivo experiments addressing the mechanisms of different PVS symptoms. The studies presented will include in vitro complement activation and cytokine release measurements in serum and blood cell cultures in vitro, attesting to proinflammatory activity of the vaccine, and anti-PEG antibody titrations in human and pig serum along with in vivo pig studies, showing a causal role of these antibodies in vaccine-induced anaphylaxis. Data will be presented on the dissemination of LNP and expression of SP all over the body due to LNP-lipid-mediated transfection of mRNA and a theory proposed on SP's similarity to bacterial superantigen toxins. The lecture will also address the broader implications of PVS and possibilities for its prevention.

**Biography:**

Dr. János Szebeni, MD, PhD, professor at Semmelweis University, CEO of SeroScience Ltd. He has held various scientific positions in Hungary and the United States. His research on various themes in hematology, and immunology resulted in over 200 publications (H-index: 60, citations ~15,000) and 2 books. Principal investigator in 12 European and Hungarian research grants and >30 CRO projects over the past 20 years. Three fields stand out where he has been most active: artificial blood, liposomes and the complement system. His original work led to the CARPA concept, i.e., that complement activation underlies numerous drug-induced (pseudo)allergic infusion reactions.

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**Safer and sustainable plastic materials by toxicity screening**

**Peter A. Behnisch** and Abraham Brouwer

*BioDetection Systems, Amsterdam, The Netherlands;*

The aims of the new European Green Deal strategy is to strengthen the economy by focusing on zero polluted and toxic-free materials by a safe and more sustainable design. Plastics in their various applications can contain a wide range of hazardous additives, as well as a large number of non-intentionally added substances (NIAS) including degradation products, processing aids or impurities in plastic additives such as e.g. brominated dibenzofurans in PBDEs. Furthermore, the recycling of plastic are a source of NIAS which can include POPs if e.g. e-waste plastic is recycled into toys. Also more and more polyhalogenated pollutants are found even in food packaging (such as PFAS) or plastic toys (such as polybrominated dioxins). Bioassays are important tools to screen a wide range of toxic effects from migration experiments and from total extracts. The complex mixtures of hundreds of additives (IAS), unknown compounds (NIAS), their transformation products and complex mixtures thereof in recycled plastic require an integrated toxicity assessment which cannot be delivered by chemical analysis of target compounds and also not by animal testing. By using effect- and human-cell based in vitro toxicity tools (such as a CALUX panel following OECD and CEN standards) for e.g., cell death, DNA damage (p53), oxidative stress (Nrf2), early warning (PXR), PFAS (thyroid hormone competition), obesity (PPAR), dioxins and endocrine disrupting properties (EATS) these known and unknown compounds can be monitored and eliminated to decrease the number of regrettable substitutions and to achieve a safer & sustainable life cycle of materials and nanomaterials.

**Biography:**

Dr. Peter A. Behnisch is Director of BioDetection Systems in Amsterdam (The Netherlands) since 2006. Since 1995 is he involved in effect-based in vitro bioassay testing of chemicals and all kinds of plastics. After his PhD in 1997 at the Eberhard-Karls University of Tübingen, Germany he also worked in several other countries such as at Lancaster University, England, at Kaneka Techno Corp. in Japan and at SGS and Eurofins in Germany. His scientific expertise is in chemical and biological analysis of all kinds of chemicals (POPs, EDCs, PFAS, BfRs) and their products. He is author from more than 100 peer-reviewed publications.

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**From coffee to green roads: a sustainable recycling of silverskin coffee wastes**

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For reducing the costs involved in the production of road pavements and to increase their lifetime, chemical additives are generally used. Nowadays attention is paid to develop green technologies, mainly based on the reduction of the use of polluting chemical substances. For this reason, bioadditives are being currently considered.

In this optics, in the seek for more sustainable processes, and to reduce CO<sub>2</sub> emissions, we have found a way to re-use the residues (oil and char) derived from ligno-cellulosic wastes pyrolysis as bitumen additives. This allows for: (i) the production of asphalts with higher performances and (ii) the recycling of wastes, and (iii) the reduction of the consumption of resources for the production of new road pavements.

This work aims to show how the products deriving from the pyrolysis of coffee silverskin, e.g. the thin layer covering the coffee beans can become added-value materials to improve the

quality of road pavements. In this contribution, we presented: (i) the physico-chemical characterization of the coffee silverskin; (ii) the

effect of silverskin (as is) on the asphalt binder (bitumen) properties and (iii) the effect of silverskin pyrolysis products (Solid -char- and liquid -oil- products,) on the bitumen characteristics. Rheological tests have been performed to determine the mechanical properties of neat asphalt binder (bitumen) and those enriched with

the coffee silverskin and its pyrolysis products. Measurements to evaluate possible anti-aging effects have been also performed. The physicochemical and thermal properties of the silverskin powder along with the determination of its microstructure were achieved by elemental analysis, Gel Permeation Chromatography (GPC), Thermogravimetric Analysis (TGA)/Derivative Thermogravimetry (DTG), Fourier Transformation Infrared



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(FTIR) spectroscopy, Scanning Electron Microscopy (SEM), Dynamic Light Scattering (DLS) and Confocal Microscopy. After the latter tests, blends with different coffee silverskin contents and char (5%, 10% and 15% by weight of bitumen) were produced. Characteristic properties such as penetration, softening point, elastic recovery, force ductility, dynamic viscosity and storage stability were determined for the reference bitumen and silverskin blends.

The collected results indicate that both coffee silverskin and char from coffee silverskin pyrolysis can strengthen/modify the bitumen and improve its mechanical properties.

### **Biography:**

Cesare Oliviero Rossi was born in 1974 in Cosenza, Italy. He is Professor at the University of Calabria. He has worked abroad as team member or research leader, running different research projects.

His publication track record, including more than 170 papers in international peer reviewed journals, is impressive. He has been focusing on the chemistry of bitumen and its additives, making use of investigation and analytical techniques never used before to study asphalt binders.

In 2015 he was awarded the gold medal for contribution to the Road Science by the High Research Institute of Kazakhstan.

## Hierarchical self-organization of Janus Nanoparticles and polymersomes for bio-applications

Voichita Mihali<sup>1,2</sup>, Piotr Jasko<sup>1</sup>, Michal Skowicki<sup>1,2</sup> and Cornelia G. Palivan<sup>1,2</sup>

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A significant approach in various fields such as chemistry, electronics, and technology is the self-organization of nano-objects into complex architectures. This strategy aims to generate novel systems with unique properties and functionalities [1–3]. An important step in creating interconnected artificial organelles is the DNA hybridization between synthetic assemblies, including polymersomes, nanoparticles, and micelles. These assemblies facilitate cascade reactions among different encapsulated catalytic compounds and can imitate cell signaling and interactions [4,5].

In this study, we explore the self-organization of clusters formed by "hard" Janus nanoparticles (JNPs) and "soft" polymersomes, presenting a universal approach to developing a hybrid system with multiple functions for specific bio-applications. The polymer-based JNPs possess anisotropic composition and orthogonally addressable functionality, making them an asymmetric platform suitable for directional interactions [6,7] with soft polymersomes. These clusters are formed through the hybridization of complementary ssDNA strands attached to each component. While adhering to the surface of the "hard" JNPs, the polymersomes undergo deformation but maintain their structural integrity due to the robustness of the block copolymer membrane. Notably, the polymersomes retain their vesicular architecture even after assembly into JNP-polymersome clusters, allowing for the encapsulation of various types of functional cargo [8]. Additionally, the biocompatibility of these clusters and their interactions with cell surfaces are facilitated by scavenger receptors. This research highlights the potential of combining "hard" and "soft" nano-objects to create multifunctional hybrid systems for advanced bio-applications.

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**Biography:**

I am a scientist with a PhD in Industrial Chemistry from the University of Milan. I have garnered significant interdisciplinary research experience in organic chemistry, polymer chemistry, Janus nanoparticles, colloids, interfaces, self-assembly of nanomaterials and DNA nanotechnology. Currently, I am a research assistant at the University of Basel, where I focus on designing artificial cells and biomimetic organelles, as well as developing self-organized bio-hybrid systems for biological applications. My work involves creating advanced functional materials through hierarchical self-organization and DNA hybridization techniques, aiming to mimic cellular structures and processes for innovative biotechnological solutions.

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**Synthesis, characterization and applications of rod-coil block copolymer:fullerene water- processable nanoparticles**

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Guido Scavia, Francesca Villafiorita-Monteleone, Stefania Zappia*

*Istituto di scienze tecnologie chimiche "Giulio Natta" SCITEC-CNR, via A. Corti 12, 20133 Milano – Italy*

The development of water-compatible nanoparticles from hydrophobic conjugated polymers represents a groundbreaking advancement with significant potential in optoelectronics, biology, and medicine. Our breakthrough lies in creating stable, water-processable nanoparticles (WPNPs) with meticulously controlled shapes and internal structures. We accomplished this by utilizing amphiphilic low band gap rod-coil block copolymers (LBG-BCPs). These WPNPs were synthesized through a modified miniemulsion<sup>2</sup> technique that eliminated the need for surfactants and substantially reduced the use of halogenated solvents. The LBG-BCPs consist of a rigid, hydrophobic p-type semiconductor polymer (such as PCPDTBT or PTB7) combined with 4-vinylpyridine (4VP)-based coil segments. This unique composition ensures the stability of the WPNPs in aqueous environments, with the 4VP coils enhancing water compatibility without requiring surfactants<sup>3</sup>. Additionally, we created semiconductor blend-WPNPs by integrating BCPs with appropriate fullerene derivatives<sup>4-6</sup>. To thoroughly characterize both WPNPs and b-WPNPs, we employed techniques such as TEM, STEM-EDX, EFTEM<sup>7</sup>, AFM, DLS, and zeta potential measurements. TEM and associated micro-analytical techniques, including STEM-EDX analysis, provided insights into the morphology and elemental distribution within particles at the nanoscale, which is crucial for understanding the self-assembly process of LBG- BCPs into WPNPs. Finally, we explored two distinct applications: i) as the active layer in Organic Photovoltaic (OPV) devices, and ii) as photosensitizers in artificial photosynthesis systems for CO<sub>2</sub> valorization.

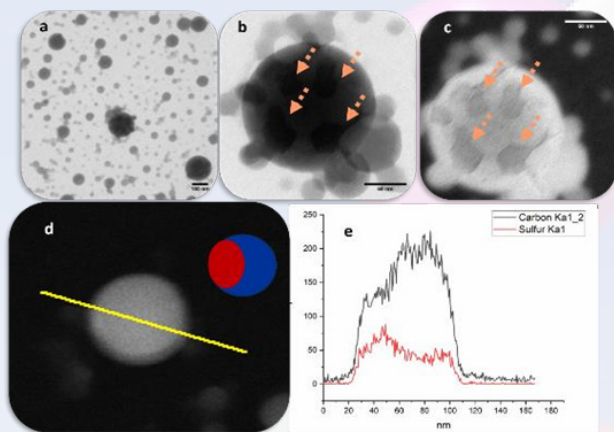


Figure a) BF-TEM images of the BCP5:PC61BM (1:3) blend NPs, b) details of one blend nanostructure c) corresponding EFTEM highlighting the area with higher concentration of PCBM. The scale bars are (a) 100 nm and (b,c) 50 nm, respectively d) STEM images of Janus WPNP, e) EDX line scan:

- 
- [1] ACKNOWLEDGEMENTS: This work was supported by Project PRIN2022- MAGnetic Inductive heating of nano- CATalyst onto metal foam as innovative approach for selective aerobic alcohol and polyol oxidation – MAGICAT - Prot. 20225RBM98, funded by the Italian “Ministero dell’Università e della Ricerca” (MUR).
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**Synthetic strategies for composite materials formed by Magnetic Nanoparticles (MNPs) and Metal Organic Frameworks (MOFs)**

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Metal organic frameworks (MOFs) are a class of materials with great interest thanks to their properties such as their facility of adopting and modifying their structure, offering precise control to select and confine different guest species. However, MOF are still in the face of various challenges and difficulties that hinder their practical application. Thus a composite material is a combination of two materials with different physical and chemical properties that when combined create a material which is specialized to do a certain job. In particular, in this work we focus on the synthesis of different MOFs compounds with magnetic nanoparticles (MNPs) of different sizes to form the new compound material.

Different synthetic methods of Fe<sub>2</sub>O<sub>3</sub> particles have been used, obtaining different particle sizes (between 4 nm and 15 nm) with different morphology. A subsequent step has been attempted to integrate magnetic nanoparticles and different MOFs into the new composite materials.

These composites were characterized by different techniques such as X-Ray powder diffraction (DRX), Raman Spectroscopy, transmission electron microscopy (TEM) and Dynamic light scattering (DLS).

**ACKNOWLEDGEMENT:**

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**Biography:**

I have a degree in Physics and a master's degree in Nanoscience and Molecular Nanotechnology. I am currently a doctoral student in the Molecular Nanoscience and Nanotechnology program. I am dedicated to the design, synthesis and characterization of new materials aimed at the elimination of emerging contaminants

7<sup>th</sup> International Conference on  
**Materials Science & Nanotechnology**  
July 15-16,2024 at Vienna, Austria (Hybrid Event)



**An alternative to photodynamic therapy via graphene-doped quantum dots**

**Paulo Cesar DE MORAIS**

*Catholic University of Brasilia, Brasilia DF Brazil*

&

*University of Brasilia, Brasilia DF Brazil*

Halogen-decorated graphene quantum dots (X@GQDs) will be herein explored as a material platform for application in photodynamic therapy (PDT). GQDs have been extensively studied in biomedical areas such as bioimaging, bio-sensing and photothermal therapy due to their superior optical and physiochemical properties. Application of GQDs in PDT has been explored lately, but currently the main challenges are inadequate singlet oxygen ( $^1O_2$ ) quantum yield (QY), poor solubility, and biocompatibility. In this talk, the synthesis of a new class of halogen (fluorine) containing GQDs (F@GQDs) will be described. The as-synthesized F@GQD sample demonstrates an average particle size below 3 nm with a fluorine doping content of around 2%. The synthesized F@GQDs show improved water solubility and biocompatibility, while emitting strong green fluorescence and QY slightly above 13%. Moreover, the photodynamic activity was successfully tested in bioassays (*in vitro*).

**Biography:**

Professor Paulo César De Morais, PhD, was full Professor of Physics at the University of Brasilia (UnB) – Brazil up to 2013. Appointed as UnB's (Brazil) Emeritus Professor (2014); Visiting Professor at the Huazhong University of Science and Technology (HUST) – China (2012-2015); Distinguished Professor at the Anhui University (AHU) – China (2016-2019); Full Professor at the Catholic University of Brasília (CUB) – Brazil (2018); CNPq-1A Research Fellow since 2010; 2007 Master Research Prize from UnB. He held two-years (1987-1988) post-doc position with Bell Communications Research, New Jersey – USA and received his Doctoral degree in Solid State Physics (1986) from the Federal University of Minas Gerais (UFMG) – Brazil. With more than 12,000 citations, He has published about 500 papers (Web of Science) and more than 16 patents.

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## **Effect of Thermocycling on the Flexure Strength of 3D-Printed Denture Materials**

**Rui Li**

*University at Buffalo, United States*

The computer-aided design/computer-aided manufacturing (CAD-CAM) systems was developed, allowing various novel materials for complete dentures fabrication. Materials used for fabrication of complete dentures using additive technology/3D-printing are being developed to overcome the shortcoming of conventional and subtractive technique, which haven shown a similar precision compared to above materials. The assessment of their accuracy, physical and mechanical are crucial so practitioners may make a decision on using various options. One of the important properties for denture base materials is their mechanical properties and a limited number of publications have reported the mechanical properties of 3D-printed denture materials. Long-term flexural strength is one of the crucial mechanical properties for complete denture base materials. High flexural strength of the denture base material allows uneven force distribution under load and resisting plastic deformation and fatigue resistance under repeated load. However, the intraoral environment is a thermally dynamic where dental materials are in contact with hot and cold beverage. Denture polymers materials in such thermal cycling may degrade due to the wet environment, while mechanical properties of the materials may reduce. Hence, it is critical to evaluate effect of thermal cycling on the mechanical properties of the acrylic resins. With new 3D-printed denture materials coming to the market there is a need for continuous assessment. This study was aimed to evaluate effect of thermal cycling on the mechanical properties of novel 3D-printed denture materials (both denture base and teeth materials). Our study found that material type, thermocycling, and their interaction significantly ( $p < 0.0001$ ) affected the flexural strength of both 3D-printed denture base and teeth materials. We concluded that 3D-printed denture base materials had a flexural strength value similar or less in comparison to milled denture base materials, and thermocycling impacted the flexural strength of denture base materials.

### **Biography:**

Dr. Rui Li, DDS, PhD, is an Assistant Professor in the Department of Restorative Dentistry, University at Buffalo, US. Dr. Li realizes the potential of emerging digital technologies in revolutionizing dental practice and patient care. She delved into the word of CAD/CAM systems, which are now standard in prosthodontics and restorative dentistry. Her Research on digital fabricated dental materials for dental prosthetics has significantly improved the precision, quality and affordability of dental restorations. She has published numerous peer-reviewed papers and abstracts in renowned dental journals and presented her findings at national/international conferences.



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**Phase change ultrasound contrast agents: new method, new opportunities**

Adam Woodward, Robert F. Mattrey, **Caroline de Gracia Lux\***

*University of Texas Southwestern Medical Center, Department of Radiology*

*Translational Research in Ultrasound Theranostics (TRUST) Program, 5323 Harry Hines Blvd, Dallas, Texas 75390-8514, United States*

With the ability to formulate stable nanodroplets (ND) of perfluorocarbon (PFC) compounds that boil below 0°C, such as perfluorobutane (PFB), acoustic droplet vaporization (ADV) of these NDs can now be achieved in vivo at acoustic energies below the FDA limit to ease clinical translation. As a result, there has been a surge of interest in ADV for theranostic applications.

In this presentation, we will talk about a robust method to produce a PFB emulsion using tools available in most laboratories, and focus on the properties of the resultant emulsion, which we show is far superior to the condensation method, the most advocated method. The dominant conclusion of our experiments (de Gracia et al. *Ultrasound in Medicine and Biology* 2023), is that nearly 100% of particles produced by direct emulsification of PFB liquid at low temperature are PFB-filled, whereas the emulsion produced by MB condensation if the MBs are not washed, contains 2000 times more non-PFB filled than PFB-filled particles. Consequently, when such suspensions are used to target receptors, the abundance of non-PFB particles will act as competitive inhibitors, and when used to extravasate to reach extravascular targets, the lower count of PFB-filled particles will require larger doses decreasing efficacy and increasing side effects. Since nearly 100% of particles will be PFB-filled with direct emulsification, it is our opinion that this formulation will yield greater efficacy at a much lower dose, which in turn will increase safety. Adopting this direct formulation could be a game changer for all applications when experimental outcome is dependent on ND concentration, stability, purity and size. As a result, this method should accelerate the translation of these ultrasound activatable NDs to both image and potentially treat diseased tissues.

**Biography:**

Dr. de Gracia Lux received her Ph.D. in Chemistry from the University of Strasbourg under the mentorship of Marie Pierre Krafft, Ph.D. synthesizing and evaluating new classes of fluorinated surfactants to promote self-assembly and compartmentalized systems for material science applications. She then completed postdoctoral training at UCSD focusing on biocompatible materials for theranostic applications.

Dr. de Gracia Lux is an Assistant Professor at UT Southwestern Department of Radiology. Her current research interest is combining creative synthetic chemistry and formulation to develop activatable ultrasound contrast agents aimed to address a wide range of challenges in cancer imaging and treatment.

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**Outstanding Hardening Effect of High-Temperature Aging of Alloy Ti-6Al-4V Composite Reinforced with TiC**

**S.V. Prikhodko**

*Department of Materials Science and Engineering, University of California Los Angeles, Los Angeles, CA 90095, USA*

Titanium alloy composites, reinforced with a light second phase and made using inexpensive powder metallurgy, attract considerable attention due to the directness of their intentional hardness increase without compromising low weight of materials. In this study the metal- matrix composites (MMC) of Ti-6Al-4V alloy reinforced with light and hard particles of TiC (up to 80%, vol.) were made using blended elemental powder metallurgy of hydrogenated titanium. Post-sintering solution treatment for 45 min at 880 °C and 1000 °C and water quenching followed by the 5 hrs. aging at 550 °C was used to additionally refine the microstructure and properties of MMC. For the duration of thermal exposure throughout solution treatment and additional aging the matrix and reinforcement phase underwent distinct structural changes that modified the mechanical properties of materials. It has been shown that the used reinforcement of the alloy with the introduced second phase and subsequent heat treatment can increase the hardness of the alloy by almost two times. Structure of MMC was characterized and properties change were explained on the base of the existing theories of hardening mechanisms in metallic systems.

**Biography:**

Currently Director of Electron Microscopy Core facilities at the Department of Materials Science and Engineering, University of California Los Angeles. Area of my scientific expertise lays in structure characterization of materials using advanced microscopies and spectroscopies including light optical, scanning electron microscopy (SEM), transmission electron microscopy (TEM), high resolution (HR) TEM, focused ion beam (FIB), dual-beam FIB-SEM, scanning transmission (ST) EM, energy dispersive spectroscopy (EDS), x-ray diffraction (XRD), x-ray microscopy, etc. Co-author of more than 100 peer-reviewed publications and more than 70 conference talks. Current research work is focused on properties of titanium alloys, titanium based composite and laminate structures.

## Measuring Dynamic Diffraction in HREM Images

Rodney A. Herring

CAMTEC, MENG, University of Victoria, British Columbia V8W 2Y2 Canada

Dynamic diffraction contributes significant contrast to high resolution lattice images adding many unknowns, the bane of quantitative imaging of crystals. Dynamic diffraction is complex, especially in strong electron scattering specimens. There hasn't been a method developed to measure the contribution of dynamic diffraction to lattice images that require thin specimen less than the extinction distance of the diffracted beams. Being able to measure its contribution would help produce better high resolution images by providing a means for its removal.

The method to measure the contribution of dynamic diffraction to lattice images was created using diffracted beam interferometry [1]. The method involves interfering two symmetrically Bragg diffracted beams on the optic axis using an electron biprism (Fig. 1a). Fig. 1b shows the interference at the [011] zone axis of the beams of aluminum by means of the electron biprism as well as the transfer of intensities from the and beams into the by dynamic diffraction. If the phase was only that of the two beams, their phases would be 100% cancelled resulting in a flat phase image. This is not the case. Instead, a residual lattice phase image is produced (Figure 2) from the dynamic diffraction of the and beams acting as new origins of diffraction during their passage through the specimen. The two beams can be considered as carrier waves of the dynamic diffraction. When interfered, the beams produce strong, high contrast fringes, Figure 2a. The phase is obtained by Fourier transform reconstruction of this interferogram revealing a weak lattice image, Figure 2b created by the interference of the and beams representing the + and + atomic planes of aluminum, Fig. 2b.

Dynamic diffraction has complex contributions to lattice images as there are many possibilities for producing it, especially for strong phase objects like gold. A complex lattice phase structure of gold is formed by the interference of its dynamically diffracted beams, Fig. 3.

Aluminum and gold representing weak and strong phase objects were used for these experiments. The lattice phase image of Al was relatively simple compared to the more complex, lattice phase image of Au. These measurements offer possibilities to help understand dynamic diffraction's contribution to HREM lattice images with the ultimate goal of being able to quantifiably determine the number and types of atoms in HREM images.

1. R.A. Herring, G. Pozzi, T. Tanji, A. Tonomura, Ultramicroscopy 60 (1995) 153. Grants from NSERC Discovery, CFI and BCKDF are greatly appreciated.

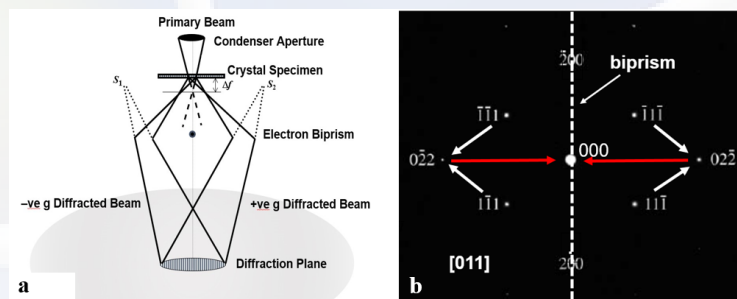


Figure 1 a) Interference of symmetrically diffracted beams by means of an electron biprism, and b) [011] diffraction pattern showing interference of diffracted beams (red arrow) by the electron biprism as well as the transfer of intensities from the  $000$  beams into the  $02\bar{2}$  beams (white arrows) causing dynamic diffraction.

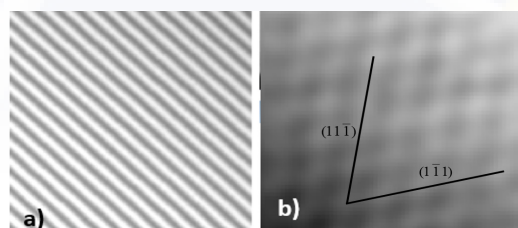


Figure 2 – a) Interferogram of Al's  $000$  and b) its reconstructed phase image revealing the  $+$  and  $+$  planes created from the interference of the  $000$  and  $02\bar{2}$  beams.

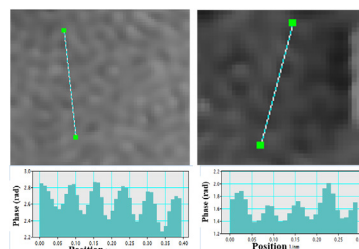


Figure 3 – a) Residual phase images of Au revealing complex periodic phase shifts due to dynamic diffraction.

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