fiRelax – Novel fitting platform for relaxivity data of paramagnetic systems

Kubrak, **Adam**; Sebastiao, Pedro; Parigi, Giacomo

Fast-Field-Cycling (FFC) NMR relaxometry offers unique insights into the molecular dynamics of paramagnetic molecules or nanoparticles through the acquisition of longitudinal relaxation rates as a function of magnetic field, the so-called Nuclear Magnetic Relaxation Dispersion (NMRD) profiles. Through model fitting with numerical algorithms, structural, dynamic and electronic parameters can be extracted, providing information on motional processes and interactions within the system. The main model used for paramagnetic NMRD profiles is the Solomon-Bloembergen-Morgan (SBM) model, whereas for systems exhibiting static Zero-Field-Splitting (ZFS), the (modified) Florence models have been developed. However, a lack of software solutions combining all paramagnetic relaxation models persists. fiRelax is a web-based fitting application featuring an intuitive graphical UI, specifically designed for the analysis of FFC data. It can be used without in-depth knowledge of programming or paramagnetic theory, and is freely accessible at https://firelax.cerm.unifi.it. The software consists of a dynamic front-end enabling analysis of experimental profiles and relaxation curve simulations, and a fitting core — the One-Fit-Engine (OFE) — where calculations and minimization procedures are performed. OFE is developed as an open-source algorithm, successfully implemented also by other fitting programs.
The platform has been tested with various datasets, including contributions from multiple relaxation processes for inner-, outer-sphere and fast internal mobility. Multiple datasets can be fit simultaneously by (1) performing fits with shared parameters or (2) using Arrhenius equations to calculate temperature dependencies.