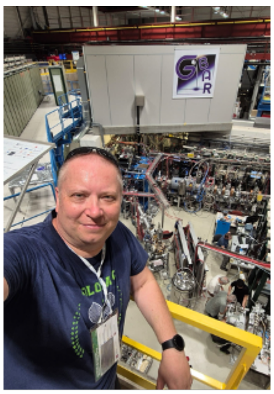
Prof. Kosma Szutkowski

NanoBioMedical Centre, Adam Mickiewicz University, Poznań

<u>Friday, Sept. 11, 2026, 11:00 am. Osborne A204</u>

Mapping Long-Range 3D Lithium Diffusion in Solid Electrolytes Using PGSE NMR, XRD, and MD Simulations. From Model Hydrides to Advanced LGPS Superionic Conductors



Solid-state lithium electrolytes are critical to the development of safe and efficient electrochemical cells. They eliminate flammable organic solvents, physically suppress dendrite growth, and significantly extend battery life for long-duration energy storage applications. Macroscopic ion transport in these materials is strictly governed by the topology, dimensionality, and local anisotropy of diffusion pathways within the crystal lattice. This lecture presents a comprehensive, multiscale research approach that integrates ^{7}Li pulsed-field gradient NMR (PGSE NMR) spectroscopy, molecular dynamics (MD) simulations, and X-ray diffraction (XRD) with Rietveld refinement.

The first part of the talk will discuss results for model hydride systems: the high-temperature hexagonal phase of $LiBH_4$ and $LiBH_4$–LiBr composites. XRD-Rietveld analysis confirmed the $P6_3mc$ space group symmetry, providing a structural basis for MD simulations, which revealed intertwined lithium migration channels along the [001] direction with zig-zag jumps across the (001) planes. PGSE NMR experiments quantified the diffusion tensor components, demonstrating distinct transport anisotropy ($D\| > D\perp$). By modeling the powder-averaged diffusion tensor based on Euclidean space rotation schemes, we derived analytical equations linking the measured spin-echo attenuation to the principal tensor components, allowing for a precise correlation between experimental activation barriers and MD energy landscapes. The focus of the lecture will be the extension of this methodology to advanced superionic sulfide conductors with an argyrodite-type structure and top-tier all-solid-state battery conductors, specifically, the LGPS ($Li_{10}GeP_2S_{12}$) family. New structural (XRD) and dynamic (^{7}Li PFG-NMR) results for LGPS phases will be juxtaposed with theoretical models to map 3D ionic percolation pathways. This integrated framework effectively opens the "black box" of macroscopic conductivity measurements, providing materials scientists with precise guidelines for optimizing crystallographic texture, lattice strain, and grain boundaries to achieve ultrafast charging in modern solid-state batteries.

Short Bio

Kosma Szutkowski obtained his PhD in Physics in 2006 at Adam Mickiewicz University in Poznań, Poland, under the supervision of Prof. Stefan Jurga. Subsequently, he was awarded a postdoctoral fellowship at KTH Royal Institute of Technology in Sweden (2006–2008), working with Peter Stilbs and Istvan Furo. He earned his habilitation in Physics in 2019. Since then, his research has centered on the applications of pulsed-field gradient NMR (PGSE NMR) for studying molecular and ionic diffusion in systems with complex architectures, including surfactant assemblies, proteins, porous materials, and polymers. Currently, his research focuses on next-generation solid-state electrolytes, combining precise experimental diffusion measurements (PGSE NMR) with molecular dynamics simulations and complementary structural methods such as X-ray diffraction XRD. Complementing his experimental work, Dr. Szutkowski actively develops custom scientific software and high-performance computational pipelines, increasingly leveraging advanced agentic AI tools to accelerate the development process. Rather than relying on off-the-shelf tools, he integrates advanced AI capabilities to design and develop custom scientific software tailored for materials analysis. Beyond his core focus on solid-state energy storage, he is an active voice in the broader energy transition and policy discourse. He regularly co-authors expert analyses on nuclear engineering with a particular focus on Small Modular Reactors (SMRs), nuclear fuel supply chains, and fusion technologies contributing a holistic perspective on global energy security.