CPP 5: Composites and Functional Polymer Hybrids

Time: Monday 11:30–13:00 Location: H38

Invited Talk CPP 5.1 Mon 11:30 H38

Theoretical characterization of sulfur/carbon copolymer cathodes for next-generation batteries via *ab initio* spectroscopy simulations — •Daniel Sebastiani and Pouya Partovi-Azar — Martin Luther University Halle-Wittenberg, Halle (Saale), Germany

The remarkable theoretical specific capacity of elemental sulfur ($\sim$1675 mAh/g) and its abundance make lithium-sulfur (Li-S) batteries an attractive alternative to current lithium-ion technology. Nevertheless, their cycle life has so far been limited due to an irreversible capacity fade. To tackle this issue, numerous studies have focused on structural optimization of sulfur cathodes including utilization of sulfur/carbon copolymers. Among others, sulfur-n-1,3-diisopropenylbenzene (S/DIB) copolymer, a 3D network of DIB molecules interconnected via sulfur chains, has shown a promising performance as an active cathode material.

In this talk, we will present our recent works employing a quantum-chemical approach for the characterization of S/DIB copolymer cathodes through simulation of their Raman fingerprints during discharge. Theoretically predicted Raman responses, calculated at density-functional theory (DFT) level along with DFT-based *ab initio* molecular dynamics simulations, hint at activities at certain frequencies which can be exploited to experimentally distinguish between the underlying structures involving short or those having longer sulfur chains. These predictions are all proven plausible by experimental Raman measurements on Li-S coin cells.

CPP 5.2 Mon 12:00 H38

Unveiling the Kinetics of Block Copolymer Micelles Close Packing by In Situ GISAXS — •Guangjiu Pan[1], Jinsheng Zhang[1], Altantulga Buyan-Arivjikh[1], Zhuijun Xu[1], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]KTH Royal Institute of Technology, SE 100 44 Stockholm, Sweden

Packing spheres has long been a key topic in science. While hard spheres often form dense, close-packed structures like face-centered cubic (FCC) lattices, soft spheres, such as block copolymers in selective solvents, tend to arrange into less dense structures. However, when using block copolymer templates in the sol-gel method, these soft spheres can achieve close-packed structures. In this study, in situ grazing-incidence small-angle X-ray scattering (GISAXS) is used to examine the self-assembly and co-assembly processes during the formation of close-packing structures. The results reveal that the hybrid films preferentially develop an FCC structure with cluster nuclei. After the polymer template is removed, a superlattice-like mesoporous metal oxide film is obtained, showcasing the potential for advanced applications due to its well-organized nanostructures.

CPP 5.3 Mon 12:15 H38

Optimizing the internal structure of soft elastic composite materials — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We study magnetic gels and elastomers, soft materials composed of magnetic or magnetizable particles embedded in a soft polymeric matrix material. These materials can be controlled by external magnetic fields, which induce deformations (magnetostriction) or changes in the rheological behavior (magnetorheological effect).

In particular, we investigate how these two effects depend on the arrangement of magnetizable particles within the elastic matrix. For the magnetostrictive effect, we consider model systems of spherical shape, for which we can analytically calculate how the volume change and overall elongation or contraction under applied magnetic fields depends on the configuration (within the linear elastic regime) [1]. Based on these formulae, we optimize the structures for maximized deformations, using an adaption of simulated annealing. Additionally, we investigate cubical systems for their magnetorheological effects, also presenting the internal arrangements that maximize these effects. The optimized arrangements are compared to regular lattice configurations.

The method that we present here can be transferred to the investigation of other types of soft elastic composite systems, driving them towards their full potential in light of future applications.

[1] L. Fischer, A. M. Menzel, PNAS Nexus **3**, pgae353 (2024).

CPP 5.4 Mon 12:30 H38

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity — •Lucas P. Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Daniel Söderberg[3], and Stephan Roth[2,3] — [1]Heinz Maier-Leibnitz-Zentrum, Technische Universität München — [2]Deutsches Elektronen Synchrotron DESY — [3]Department of Fibre and Polymer Technlogy, KTH Royal Institute of Technology

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is a conductive polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water ($\approx$50 V%), causing swelling, degradation, and eventually a decrease in conductivity. Integrating PEDOT:PSS with cellulose nanofibrils (CNFs) overcomes these issues by limiting water absorption and enhancing mechanical stability. However, in humid environments, a minor amount of water is still absorbed, leading to a change in film morphology: the absorbed water induces de-wetting of PEDOT:PSS from the CNFs, reducing conductivity, whereas drying generally leads to a re-wetting of PEDOT:PSS, thereby restoring conductivity. To investigate further the role of water, quasi-elastic neutron scattering is applied, which reveals two water species in the films: mobile bulk water and slower hydration water. Upon drying, bulk water is released completely, while hydration water remains in the films, supporting the re-wetting of PEDOT:PSS. QENS also provides information on the diffusive and hydrogen-bonding behavior of water.

CPP 5.5 Mon 12:45 H38

Enhanced Physical Properties and Shape Recovery in Epoxy-Based Shape Memory Polymer Nanocomposites under Gamma Irradiation for Aerospace Applications — •Eman Taha — 1 Ahmed El-Zomor St, 11727, Cairo, Egypt.

This research explores the impact of gamma irradiation on the structural and functional properties of epoxy-based shape memory polymer nanocomposites, specifically engineered for potential satellite deployment mechanisms in space applications. To enhance durability and adaptability in extreme conditions, multi-walled carbon nanotubes (MWCNTs) were incorporated into the epoxy matrix, with surfactants added to improve dispersion. Using a Cobalt-60 gamma irradiation facility, doses ranging from 250 to 1000 kGy were applied, uncovering dose-dependent changes in thermal stability and mechanical properties. Surface tension tests confirmed effective dispersion with nonionic (Tween 80) and anionic (SDS) surfactants, while cationic surfactants had less impact. Thermogravimetric analysis revealed enhanced thermal stability at moderate doses due to increased crosslinking. Dynamic mechanical analysis showed shifts in viscoelastic behavior and higher glass transition temperatures (Tg), critical for thermal stress resistance. Shape memory performance improved at 250 kGy but declined at higher doses, indicating a balance between radiation exposure and functionality. These findings highlight controlled gamma irradiation as a tool to optimize the performance and stability of epoxy-based nanocomposites with MWCNT reinforcement, advancing their suitability for space applications.