CPP 41: Charged Soft Matter, Polyelectrolytes and Ionic Liquids II

Time: Wednesday 15:00–15:30 Location: H13

CPP 41.1 Wed 15:00 H13

Neutron reflectivity and MD simulations of the silicon - deep eutectic solvent interface — •Nebojša Zec[1], Gaetano Mangiapia[1], Sebastian Busch[1], and Mikhail Zheludkevich[2] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ) Helmholtz-Zentrum Geesthacht GmbH, 85748 Garching bei München, Germany — [2]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany

The main aim of this work is to reveal the structure of the layers formed at the interface between deep eutectic solvents (DES) and silicon surface with and without applied constant electric potential using neutron reflectometry (NR) and molecular dynamics simulations (MDs). Work is focused on finding experimental evidence for an ordered layer of DES over an Si substrate under DC conditions and resolving the destruction of this layer by a superimposed AC field. Electrochemical experiments have shown that application of the potential of -1.6V superimposed with alternating sinusoidal component of 50 mV allows zinc depostion. Increasing temperature has the same effect and at 100 degrees C electrodeposition is possible even in potentiostatic regime. The results obtained with REFSANS instrument at Heinz Maier-Leibnitz Zentrum (MLZ) are compared with the reflectivity calculated from molecular dynamics simulations. Through this work we tend to determine the relationship between NR measurements of DES/silicon interface and the corresponding structural information obtained by MD simulations of the same system.

CPP 41.2 Wed 15:15 H13

Self-assembly of hollow colloidal silica cubes — •Margaret Rosenberg[1], Frans Dekker[2], Joe G. Donaldson[1], Albert P. Philipse[2], and Sofia S. Kantorovich[1,3] — [1]Department of Physics, University of Vienna, Vienna, 1090, Austria — [2]Van't Hoff Laboratory for Physical and Colloid Chemistry, Debye Institute for Nano-Materials Science, Utrecht University, NL — [3]Department of Mathematical Physics, Ural Federal University, Russia

Among the multitude of recently synthesized non-spherical colloids, hollow silica cubes distinguish themselves by their charged surface and the strong influence of van der Waals forces on their behaviour. While their self-assembly has been observed in experiment, it has not yet been fully studied and characterized. Using MD simulations, we investigate the electric double layer surrounding the cubes, then compute their interaction potential at different orientations to understand the influence of their anisometry. In combination with experimental observations and calculated trajectories, we show how the self-assembly of the cubes is driven by the competition between electrostatic and van der Waals forces. We then examine the microstructures formed by small clusters of cubes, which differ significantly from those exhibited by comparable spheres. These investigations give us a multifaceted understanding of the behaviour observed in these systems and pave the way for future applications.