CPP 14: French-German Session: Simulation Methods and Modeling of Soft Matter II

Time: Monday 17:15–19:00 Location: ZEU/LICH

CPP 14.1 Mon 17:15 ZEU/LICH

Lateral interactions in Bisphenol A adsorption on Carbon Nanotubes — •Oliver Cunningham and David Wilkins — Queen's University Belfast, Belfast, Northern Ireland

Endocrine disrupting chemicals (EDCs) such as Bisphenol A (BPA) are being found in water supplies with increasing frequency and our methods of water treatment need to improve alongside this ever increasing problem to mitigate the risks they pose to human health. Molecular Dynamics paired with enhanced sampling methods such as Metadynamics have proven to be very effective at studying the free energy profiles for processes like adsorption. To this end we present the effects lateral interactions between BPA molecules have on their adsorption onto a single walled carbon nanotube (SW-CNT) and how this depends on the number of BPA. The free energy of adsorption is studied as it gives insight into how well a SW-CNT adsorbs BPA and therefore how effective it is at removing it from water. Studying the free energy of adsorption for systems with varying numbers of BPA, we find that the free energy of adsorption increases with the number of BPA. This shows that lateral interactions between BPA molecules have a noticeable effect on how well they adsorb on the surface. We find two free energy minima corresponding to different conformations of the BPA, and the energy barrier between these minima decreases with the number of BPA. We also show that Parallel Bias Metadynamics provides an efficient way to bias all of the BPA in a system, providing better statistics than individually biased runs, while still achieving free energy's adsorption in agreement with the individual runs.

CPP 14.2 Mon 17:30 ZEU/LICH

Multiscale Modeling of Grain Boundary Effects on Charge Transport in Pentacene — •Sonali Garg, Farhad Ghalami, and Marcus Elstner — Karlsruhe Institute of Technology, Karlsruhe, Germany

Organic semiconductors have emerged as crucial materials in the development of electronic and optoelectronic devices due to their exceptional mechanical flexibility, lightweight nature, and cost-effectiveness. However, the presence of grain boundaries (GBs) can significantly impede device performance by introducing structural defects that affect charge-carrier movement and reduce mobility. In this study, we developed a model to investigate the influence of GB characteristics, including misorientation angles and GB width, on charge carrier mobility, and compare the results with intrinsic mobility. Non-Adiabatic Molecular Dynamics (NAMD) simulations, employing the Fewest Switches Surface Hopping (FSSH) approach[1,2,3] were used to model charge transport dynamics. The charge transfer Hamiltonian was constructed using a fragment orbital approach, with its elements computed via the Density Functional Tight Binding (DFTB) method[4,5]. These insights provide a deeper understanding of the effects of GBs on charge-carrier mobility in organic semiconductors.

[1]Spencer. J et al. J. Chem. Phys. (2016) [2]Roosta. S J. Chem.Theory Comput. (2022) [3]Xie. W et al. J. Chem Theory Comput.(2020) [4]Elstner. M et al. Phys. Rev. B (1998) [5]Kubař. T et al. J.Phys. Chem. B (2010)

CPP 14.3 Mon 17:45 ZEU/LICH

A classical model to describe the electric potential-dependent water structure at metal interfaces — •Damien Toquer[1], Henrik Stooss[1], Philipp Stärk[1,2,3], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [3]SC Simtech, University of Stuttgart, 70569 Stuttgart, Germany

Nano- and microfabrication enable the development of functional materials tunable across length scales. While atomistic simulations are a powerful tool for studying and designing such materials bridging atomic-to-macroscopic properties remains challenging. The electrode/water interface exemplifies this challenge, explicit electronic treatment limits simulation scalability. Various schemes have been proposed that aim to incorporate metallic electronic response into classical molecular dynamics. Recently, the constant potential method has shown promise, where charges are attached to the metal atoms to maintain a fixed electrode potential. Our goal is to develop an efficient classical model that reproduces interfacial water structure across various electrode potentials, using gold surfaces as a prototype. Gold charges are adjusted to capture long-range continuum electrostatic interactions, while short-range interactions are tuned to match ab initio energy calculations. We anticipate this model will reliably predict interface-dependent thermodynamic properties both at equilibrium and under applied electrode potential, and plan to use it to study electrowetting in parallel with experimental work.

CPP 14.4 Mon 18:00 ZEU/LICH

Acoustic Effects in Electrolytes with Interfaces: Mechanistic Insights from MD Simulations — •Katharina Kintrup[1], Youssef Mabrouk[1,2], Diddo Diddens[1,3], and Andreas Heuer[1] — [1]Universität Münster, Institut für Physikalische Chemie, Deutschland — [2]Friedrich-Schiller-Universität Jena, Institut für Physikalische Chemie, Deutschland — [3]Helmholtz-Institut Münster, Deutschland

Interfaces such as electrodes strongly affect transport and dynamics in electrolytes. However, Molecular Dynamics (MD) simulations often assume periodic boundary conditions (pbc), thereby neglecting interfacial effects. This enforces a fixed center-of-mass frame in simulations, whereas electrophoretic NMR (eNMR) experiments [1,2] have shown that, in laboratory electrolytes, the center of mass drifts and local volume conservation is the appropriate assumption.

To mimic laboratory conditions, we introduce explicit interfaces in MD simulations and employ external fields for comparison with eNMR. As expected, we also observe a drift of the center of mass, but we do not find ideal local-volume conservation. Instead, we obtain oscillatory signals that reveal a strong dominance of acoustic effects over the intrinsic ionic dynamics. For binary electrolytes, we formulate a theoretical description that accurately incorporates the finite compressibility of the fluid. Overall, our work provides spatial and temporal insights into electrolyte dynamics in the presence of interfaces and highlights the importance of the chosen reference frame. [1] J. Phys. Chem. Lett. 2022, 13, 37, 8761-8767; [2] ACS Appl. Polym. Mater. 2025, 7, 13, 8432-8444

CPP 14.5 Mon 18:15 ZEU/LICH

Understanding electrode/electrolyte interfaces for electrocatalysis using constant potential DFT simulations — •Henrik Stooss[1], Philipp Stärk[2], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg University of Technology, 21071 Hamburg — [2]Institute for Computational Physics, Universität Stuttgart, 70569 Stuttgart

This study explores the complex dynamics at electrode/electrolyte interfaces under constant potential, which is crucial for advancing electrocatalysis and designing efficient energy systems. We combine advanced computational techniques to gain insights into the mechanisms at these interfaces. Specifically, we perform Density Functional Theory (DFT) simulations of interfacial systems while maintaining a constant electrode potential. Despite the associated challenges and computational costs, these simulations provide valuable insights into the electronic structure and behavior of electrode surfaces. We calculate IR spectra of water in front of a gold electrode at different applied potentials and compare the results with experimental ATR-SEIRAS data, thereby strengthening the connection between first-principles calculations and experimental observations for material design.

CPP 14.6 Mon 18:30 ZEU/LICH

Atomistic modeling of azopolymers: light-induced deformation — •Dmitry Ryndyk[1,2], Olga Guskova[1], and Marina Saphiannikova[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Technische Universität Dresden, Germany

In our recent study [1], we employ, for the first time, a fully atomistic force-field approach to model light-induced deformations in side-chain azopolymers. To mimic sample illumination, we introduce an orientation potential that reorients the azo chromophores perpendicular to the light polarization direction. This strategy enables us to capture both the microscopic details of chromophore behavior and the collective, anisotropic response of the polymer matrix. The atomistic simulations show a clear correlation between chromophore reorientation and sample contraction, as well as between backbone alignment and sample elongation. The separation of time scales between these two processes is controlled by the relative distance to the glass-transition temperature. Furthermore, the simulations elucidate a role of the flexible spacer in transferring the light-induced torque to the polymer backbone.

[1] D.A. Ryndyk, O. Guskova, M. Saphiannikova, Light-induced deformation of side-chain azo-polymer: Insights from atomistic modeling, arXiv:2511.19787 (2025)

CPP 14.7 Mon 18:45 ZEU/LICH

Self-Assembly of Porphyrin-Based Monomers into Supramolecular Polymers — •Mira Mors[1], Hanna Rieger[2], Oliver Stach[2], Thomas Speck[1], and Pol Besenius[2] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Germany — [2]Department of Chemistry, Johannes Gutenberg-University Mainz, Germany

Through a combination of computational modeling and experiments, we investigate the assembly pathways of water-soluble supramolecular porphyrin-peptide amphiphiles. Our computational approach employs a coarse-grained, nine-bead planar model that captures the essential molecular interactions. Simulations show that stronger interactions promote polymerization, whereas increased monomer flexibility hinders it, consistent with experiments in which an additional glycine is introduced into the peptide arms. The observed power-law dependence of the polymerization half-time suggests a nucleation-elongation-aggregation pathway; however, experiments show no concentration-dependent aggregation. To probe oligomer stability, we apply a simplified free energy model and enhance sampling by generating a grand canonical system to map free energies across cluster sizes. Aggregation kinetics are additionally studied by solving the rate equations explicitly and using moment-based approaches. These analyses reproduce the dynamics from low to high interaction strengths, highlighting the vital role of recombination in the polymerization regime. Overall, our results provide a framework for a better understanding of supramolecular polymerization under varying conditions.