CPP 3: French-German Session: Membranes and Porous Materials I

Time: Monday 9:30–11:00 Location: ZEU/LICH

Invited Talk CPP 3.1 Mon 9:30 ZEU/LICH

Theory and Modeling of Fluid Adsorption and Transport in Nanoporous Materials — •Benoit Coasne — CNRS/University Grenoble Alpes, Grenoble, France — Institut Laue-Langevin, Grenoble, France

Nanoporous materials are at the heart of numerous important applications: adsorption (gas sensing, chromatography), energy (hydrogen storage, fuel cells and batteries), environment (phase separation, water treatment, nuclear waste storage), etc. Among these materials, nanoporous solids which have pores of the order of nm (e.g. active carbons, zeolites), are particularly interesting as ultraconfinement in their porosity leads to novel adsorption and transport phenomena. In this talk, we will present how molecular simulation and statistical physics allows developing models for adsorption and transport in these extremely confining materials. We will see how simple thermodynamic modeling allows rationalizing adsorption by considering reminiscent capillarity at vanishing lengthscales. Then, we will show how transport in nanoporous media can be described without having to rely on macroscopic concepts such as hydrodynamics. In particular, using parameters and coefficients available to experiments, we will see how transport coefficients can be rigorously upscaled using simple models such as intermittent brownian motion and free volume theory.

CPP 3.2 Mon 10:00 ZEU/LICH

Optimizing the Fabrication of Isoporous Block Copolymer Membranes by Concurrent Multi-fidelity Simulations — •Gregor Häfner and Marcus Müller — Institute for Theoretical Physics, University of Göttingen, Germany

Integral-asymmetric copolymer membranes promising promising class of functional macromolecular systems with diverse potential applications, including water purification and protein separation. Their fabrication is a two-step process: solvent evaporation and subsequent nonsolvent-solvent exchange to create an isoporous top-layer, and a spongelike substructure. We model the process using two complementary schemes – a highly coarse-grained, particle-based model that treats the polymer chains directly, and a continuum model, describing the system only by its concentration fields. To exploit the accuracy of the former while retaining the efficiency of the latter, we couple these for a concurrent multi-fidelity simulation. The continuum simulation treats the whole system, spawning a particle-based simulation in the region of its lowest accuracy. For this, a neural network is employed to estimate the future error and guide the decision of the subdomain position. We achieve a tenfold increase in computational efficiency compared to pure particle-based simulations, enabling us to investigate large film depths. Our simulations delineate a process window for successful membrane fabrication, which fully match the experimentally accessible parameters, showing an isoporous top layer, a porous substructure and finger-like macrovoids, allowing us to guide experimental membrane optimization.

CPP 3.3 Mon 10:15 ZEU/LICH

In situ monitoring of relaxation dynamics in polyethylenimine during CO2 absorption and desorption — •Martin Tress — Peter Debye Institute for Soft Matter, Leipzig University

Chemical reactions between carbon dioxide (CO2) and amine have been extensively characterized, however, their influence on the dynamics of polyamines remains largely unexplored. In this work, we compare the dynamics of polyethylenimine (PEI) before and after CO2 absorption through broadband dielectric spectroscopy (BDS) [1]. Upon CO2 absorption, thin film PEI shows a slower dynamics, which is consistent with an elevated glass transition temperature revealed in complementary differential scanning calorimetry measurements. Insitu kinetics measurements in thin film samples as well as PEI-infused porous silica demonstrate complex changes in the overall permittivity as well as relaxation times and relaxation amplitudes of some processes during CO2 sorption or desorption. This suggest an intriguing interplay between physical and chemical CO2-sorption, diffusion and the dynamics of PEI. Finally, a tentative model will be presented to describe the observed curves qualitatively. These results demonstrate that BDS is a powerful in-situ-platform to resolve the temporal dynamical changes of polyamines and their impact on sorption kinetics, and may inform specific system adjustments to improve CO2 capture performance.

[1] M. Tress, S. Ahmadi and S. Cheng, AIChE J. 71 (2025) e18627

CPP 3.4 Mon 10:30 ZEU/LICH

Scalable and Tunable Carbon Nanomembranes for Selective Molecular Transport — •Zhen Yao[1], Jan Biedinger[1], Martin Wortmann[1], Nikolaus Meyerbröker[2], Yang Yang[1], Andreas Hütten[1], Günter Reiss[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Bielefeld, Germany — [2]bCNM Technologies GmbH, Bielefeld, Germany

Carbon nanomembranes (CNMs), molecularly thin two-dimensional materials with intrinsic sub-nanometer pores, provide a versatile platform for nanofluidics. Their ultrathin structure enables fast molecular flux, while surface chemistry and pore architecture can be tailored for selective transport. We present a scalable synthesis route based on electron-induced crosslinking of spin-coated poly(4-vinylbiphenyl) films, combined with atomic layer deposition (ALD) for pore and surface functionalization. This strategy enables precise tuning of pore dimensions and hydrophilicity, yielding CNMs with water vapor permeance as high as 1.9×10^{-5} mol s^{-1} m^{-2} Pa^{-1} and H_2O/N_2 selectivity above 10000, outperforming state-of-the-art polymer and graphene oxide membranes. These results establish CNMs as promising candidates for energy-efficient dehumidification and gas separation. Together, these studies demonstrate how scalable fabrication and nanoscale interface engineering translate into tunable nanofluidic transport, highlighting CNMs as a versatile materials platform for separations, sensing, and controlled molecular flow.

CPP 3.5 Mon 10:45 ZEU/LICH

Is it possible to use nano-confined water for cloaking or magnifying of static electric fields? — •Kira Fischer[1], Julia Brandt[1], Philipp Stärk[2], Alexander Petrov[1], and Alexander Schlaich[1] — [1]Hamburg University of Technology — [2]University of Stuttgart

Assuming radial anisotropy in the dielectric response of water in cylindrical or spherical confinement, Kettunen et al., have shown that for certain ratios of permittivity contrast it is possible to cloak the interior sample, or to magnify the response of an inner cylinder. Indeed, water at interfaces and in confinement shows a strongly anisotropic dielectric response, with high dielectric permittivity in parallel and low permittivity perpendicular to the interface, as observed experimentally by Fumagalli et al.

Here, we probe the radial and azimuthal dielectric response of water in cylindrical confinement. We do so by calculating the dielectric permittivity profile from molecular dynamics simulations, both using a Green-Kubo relation as well as applied fields. Near the interface, we observe a high dielectric permittivity in the azimuthal direction and a low dielectric permittivity in the radial direction of the cylinder, supporting the concept of radial anisotropy.

Applying a static, homogenous external field we then analyse the resulting water polarization. The observed effective response of water inside a cylinder is almost bulk like, and no significant cloaking effect is observed. We use effective medium theory to rationalize this behavior and discuss possible applications of cloaking in model fluids.