Seminar/Talk

Grafting heterogeneities rule intrusion and extrusion in nanopores

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Hydrophobic nanoporous materials resist water intrusion due to confined spaces and hydrophobicity, requiring pressure to force water in. In these conditions, water enters the nanopores only under pressure, and vapor bubbles must nucleate to cause the opposite phenomenon of extrusion, which typically occurs at lower pressures1. Controlling intrusion/extrusion (IE) hysteresis is crucial for applications like energy materials, high-performance liquid chromatography, and liquid porosimetry2, yet its molecular mechanisms remain unclear.We develop a coarse-grained (CG) model of a functionalized silica nanopore to investigate how surface heterogeneities influence IE. While atomistic simulations often employ smooth hydrophobic surfaces, our model explicitly accounts for organosilane grafting.Molecular Dynamics simulations reveal how small variations in graftingsuch as chain length and densitysignificantly impact IE, modifying pressures, their abruptness, and energy dissipation. Local variations in pore radius and contact angle, induced by grafting heterogeneities, can pin water, shifting IE pressures by up to 60 MPa and doubling energy dissipation.This CG approach bridges microscopic structure and macroscopic behavior, offering new insights into the design of energy materials, chromatography columns, and porosimetry analysis. We are extending the model to more realistic geometries and pore networks, closing the gap between idealized single-pore models and complex porous matrices while maintaining sub-molecular resolution.(1) Giacomello, A. et al., Eur. Phys. J. B 2021.(2) Fraux, G. et al., Chem. Soc. Rev. 2017.

Thursday, March 27, 2025 11:00am - 12:00pm
Office Bldg West / Ground floor / Heinzel Seminar Room (I21.EG.101)

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