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Surface interactions and reactions strongly impact ion adsorption and electrokinetic transport

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Detailed insight into the structure and electrokinetic transport of electrolyte solutions in nanoconfinement is hard to obtain. Experimental techniques are often either limited in their accessible resolution or their interpretation relies on models and assumptions that may not hold in nanoconfinement. Molecular simulations can in principle provide such insights, but the simulation results depend sensitively on the model input. Consequently, both the experimental and computational literature contains various contrasting data.

In my talk, I will focus on two aspects of simulating nanoconfined electrolytes. First, I will present an effective method to use unambiguously interpretable experimental data to tune simulation input and I will use these simulations to provide new insight into the coupling between ion adsorption and transport [1].

Second, I will present a method that allows the surface charge distribution on a non-conducting material to evolve in time, thus mimicking the effect of surface reactions in chemical equilibrium [2]. Such reactions are universally assumed to have no notable influence on interfacial fluid properties, regardless of the simulation time, surface material, or temperature considered. Our simulations show that accounting for surface reactions can strongly and qualitatively affect ion adsorption and electrokinetic properties.

Participation

In-Person

References

[1] M.F. Döpke and R. Hartkamp, “The importance of specifically adsorbed ions for electrokinetic phenomena: bridging the gap between experiments and MD simulations” J. Chem. Phys. 154 094701 (2021)

[2] M.F. Döpke, F. Westerbaan van der Meij, B. Coasne, and R. Hartkamp, “Surface protolysis and its kinetics impact the electrical double layer” Phys. Rev. Lett. 128, 056001 (2022)

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