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Examining Permittivity Effects in Electric Double Layers using Molecular Dynamics and Atomistic-to-Continuum Modeling JEREMY TEMPLETON, KRANTHI MANDADAPU, JONATHAN LEE, REESE JONES, JONATHAN ZIMMERAN, Sandia National Laboratories — Charged surfaces exposed to an ionic solution attract an electric double layer: stratifications of solvent and solute molecules significantly deviating from their bulk concentrations. The double layer screens the charges in solution from those at the surface, but due to the anisotropy in the near-wall fluid, characterizing the precise mechanics by which this happens has proven difficult. Molecular dynamics (MD) simulations are capable of explicitly resolving the complex layering effects in the vicinity of the charged interface, but much work remains to analyze the results and improve the understanding of these phenomena. In this work, we use atomistic-to-continuum methods to analyze the spatially-varying electrical permittivity in these layers at different potentials and ion concentrations, focusing on salt water solutions. The permittivity is a particularly relevant quantity because it determines the capacitance of the different ionic layers. We will present a mathematical formalism for extracting this quantity from an MD realization and provide examples of how this coarse-grained quantity varies with a simulation. It will then be demonstrated how the resolved permittivity informs the realized voltage drop across the various parts of the double layer.

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