

Abstract Submitted
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Molecular Dynamics Models of the Electric Double Layer for Large Zeta Potentials JONATHAN W. LEE, Sandia National Laboratories, JEREMY A. TEMPLETON, ROBERT H. NILSON, STEWART K. GRIFFITHS, BRYAN M. WONG, ANDY KUNG — The Classical Poisson-Boltzmann (PB) theory for the electric double layer (EDL) breaks down at the nanoscale as zeta potential increases. The ability to accurately model the EDL for large potentials is important for engineering high energy storage devices. To better understand behavior at large potentials, various molecular dynamics (MD) models were developed. MD models range from an idealized Lennard-Jones ionic fluid between unstructured walls to a salt water solution between solid substrates. All models feature a bulk fluid region in order to obtain a reference state. Models are compared using charge density profiles, solvent and solute concentration profiles, and zeta potentials as metrics. Local polarization structure can be obtained from the salt water MD models. Despite its inability to capture these effects, the idealized model similarly deviates from PB theory at large potentials. Ion concentration and surface charge density are varied in a parametric study using the idealized model.

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