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Electric Double Layer Structures near Rough Surfaces: Molecular Dynamics Simulation DAEJOONG KIM, ERIC DARVE, Stanford University — S. S. Dukhin in Surface and Colloid Science (1974) mentioned both the possibility of increase in zeta potential due to surface roughness and the possibility of decrease, depending on Debye length relative to surface roughness. In this work we report our results of molecular dynamic (MD) simulations on electric double layer structures near solid surfaces having roughness with the order of magnitude of Debye length. For computational simplicity only counter-ions are present. We computed static and dynamics properties including density profiles of water and ions, electrostatic potential distributions due to ions, polarization density profiles and self-diffusivities of water and ions. We also performed nonequilibrium MD to simulate electroosmotic flows. From electrostatic potential distributions and slip plane locations, we computed zeta potential and found that it decreases with surface roughness. It also showed a dependency on the spatial frequency of surface roughness. For comparison we used the Helmholtz-Smoluchowski relation and found the same trend. Currently we are studying pressure-driven flows, a computational counterpart to streaming current experiments. One of the purposes is to find more exact locations of slip planes by fitting to Poiseuille flow solutions. We are also simulating model systems with co-ions to investigate the possibility of charge inversion and other effects.

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