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Atomistic Molecular Dynamics Simulations of the Electrical Double[1] ZIFENG LI, SCOTT MILNER, KRISTEN FICHTHORN, Penn State University — The electrical double layer (EDL) near the polymer/water interface plays a key role in the colloidal stability of latex paint. To elucidate the structure of the EDL at the molecular level, we conducted an all-atom molecular dynamics simulations. We studied two representative surface charge groups in latex, the ionic surfactant sodium dodecyl sulfate (SDS) and the grafted short polyelectrolyte charged by dissociated methyl methacrylic acid (MAA) monomers. Our results confirm that the Poisson-Boltzmann theory works well outside the Stern layer. Our calculated electrostatic potential at the Outer Helmholtz Plane (OHP) is close to the zeta potential measured experimentally, which suggests that the potential at the OHP is a good estimate of the zeta potential. We found that the position of the OHP for the MAA polyelectrolyte system extends much further into the aqueous phase than that in the SDS system, resulting in a Stern layer that is twice as thick. This model will allow for future investigations of the interactions of the surface with different surfactants and rheology modifiers, which may serve as a guide to tune the rheology of latex formulations.

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