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Ion distributions near dielectric interfaces from Car-Parrinello molecular dynamics[1] VIKRAM JADHAO, Northwestern University, FRANCISCO SOLIS, Arizona State University, MONICA OLVERA DE LA CRUZ, Northwestern University — Free charges in media characterized by different dielectric constants and separated by thin boundaries are basic models for studying phenomena in both biological and synthetic materials. Knowing the distributions of ions near the dielectric interfaces between these media is crucial towards understanding the structural and physical properties of these systems. We present a new Car-Parrinello molecular dynamics method for simulating charges in heterogeneous media and computing such distributions. This method is founded on a true energy functional of induced charge density which enables the replacement of the expensive solution of the Poisson equation at each simulation step with an on-the-fly computation of polarization effects. Our simulations track the exact induced density at all times and demonstrate excellent energy conservation. The method is applied to study models of a charged colloid in polar solvent, ions near a liquid-liquid emulsion droplet, and charged biological macromolecule in aqueous solution. Results for ionic density profiles for different dielectric contrasts, ion concentrations, ion valencies, and different interfacial shapes are presented.

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