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Ion distributions in electrolyte confined by multiple dielectric interfaces YUFEI JING, JOS W. ZWANIKKEN, VIKRAM JADHAO, MONICA DE LA CRUZ, Department of Material Science Engineering — The distribution of ions at dielectric interfaces between liquids characterized by different dielectric permittivities is crucial to nanoscale assembly processes in many biological and synthetic materials such as cell membranes, colloids and oil-water emulsions. The knowledge of ionic structure of these systems is also exploited in energy storage devices such as double-layer super-capacitors. The presence of multiple dielectric interfaces often complicates computing the desired ionic distributions via simulations or theory. Here, we use coarse-grained models to compute the ionic distributions in a system of electrolyte confined by two planar dielectric interfaces using Car-Parrinello molecular dynamics simulations and liquid state theory. We compute the density profiles for various electrolyte concentrations, stoichiometric ratios and dielectric contrasts. The explanations for the trends in these profiles and discuss their effects on the behavior of the confined charged fluid are also presented.

Yufei Jing
Department of Material Science Engineering

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