Ionic Structure in Liquids Confined by Dielectric Interfaces

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We compute the ionic structure in a model system of electrolyte confined by two planar dielectric interfaces using molecular dynamics (MD) simulations and liquid state theory. We explore the effects of high electrolyte concentrations, multivalent ions, dielectric contrasts, and external electric field on the ionic distributions. We observe the presence of non-monotonic ionic density profiles leading to a layered structure in the fluid which is attributed to the competition between electrostatic and steric (entropic) interactions. We find that thermal forces that arise from symmetry breaking at the interfaces can have a profound effect on the ionic structure and can oftentimes overwhelm the influence of the dielectric discontinuity. The combined effect of ionic correlations and inhomogeneous dielectric permittivity significantly changes the character of the effective interaction between the two interfaces.