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Electrolyte-mediated adsorption to neutral and dielectric interfaces JOS ZWANIKKEN, University of Massachusetts, Lowell, YUFEI JING, Northwestern University, VIKRAM JADHAO, Johns Hopkins University, MONICA OLVERA DE LA CRUZ, Northwestern University — Biology relies on electrolytes to regulate molecular interactions and to support functionality in numerous vital processes. Although the role of the electrolyte is generally categorized into two tendencies, namely "salting-out" and "salting-in", the more versatile aspects can be revealed by a more detailed picture of the microscopic ionic structure. We use molecular dynamics simulations and numerical calculations based on liquid state theory, and obtain high-resolution, quantitative information about the spatial structure of primitive model electrolytes in dielectric confinement, up to high concentrations (0.9 M) and strong electrostatic coupling. The theoretical methods also quantify two relevant underlying thermal forces that are highly tunable by the specific selection of electrolytes. The results refine the understanding of the adsorption behavior of ions and macromolecular solutes, and identify tuning parameters for macromolecular assembly, based on ion size, valency, and ionic composition.

Jos Zwanikken
University of Massachusetts, Lowell

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