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A density functional approach to model highly charged spherical colloids in electrolyte mixtures BHARAT MEDASANI, ZAVEN OVANESYAN, MARCELO MARUCHO, University of Texas at San Antonio — We present a classical density functional (DFT) approach to study the effects of ion size asymmetry, ion-ion correlation and solvent excluded volume on the structural and thermodynamic properties of strongly interacting charged systems. The hard sphere correlation effects are modeled non-perturbatively with weighted density approximation, where as electrostatic correlations are modeled perturbatively within the mean spherical approximation. The present DFT approach is able to describe macro-ions in electrolytes comprising neutral hard sphere mimicking water molecules and ions with dissimilar valence and realistic sizes and densities. We applied the theory to study spherical electric double layers and obtained results in good agreement with simulations. We calculated ion profiles, integrated charge, mean electrostatic potential, ionic coordination number, zeta potential, and inverse differential capacity at different conditions. For higher surface charge on macromolecule, charge inversion is noticed and when the counter-ions are bigger than co-ions, surface charge amplification is observed. Layering and screening effects are more pronounced when water molecules are explicitly considered. This work has potential applications in bio-electrostatics and colloidal engineering.

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