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Field-theoretic Formulation of Ion Correlations with Explicit Hard-Core Size in Aqueous and Non-Aqueous Electrolytes

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The accurate formulation of ion correlations in charged solutions is a critical task for the control of various biological and industrial processes ranging from ion transport through cells to water purification procedures. The theoretical tools enabling the comprehension of these systems is based on the Debye-Hückel (DH) theory suffering from major limitations [1]. Namely, the validity of the DH formalism neglecting the ionic hard-core (HC) size and including exclusively electrostatic weak-coupling-level ion correlations is limited to the characterization of monovalent salts at dilute concentrations.

In this talk, I will present an ion size-augmented self-consistent DH (SCDH) theory of bulk electrolytes exploiting the asymmetric incorporation of the short- and long-range ion interactions via their virial and cumulant-level treatment, respectively [2,3]. The underlying variational splitting of the distinct interaction ranges enables the accurate prediction of ionic activity coefficients,
internal energies, osmotic pressures, and radial distribution functions of aqueous and non-aqueous electrolytes up to molar salt concentrations.

[1] P. Debye and E. Hückel, “The theory of electrolytes. I. Lowering of freezing point and related phenomena”, Zur Theorie der Elektrolyte. Phys. Z. 24, 185 (1923).
[2] S. Buyukdagli, “Self-consistent electrostatic formalism of bulk electrolytes based on the asymmetric treatment of the short- and long-range ion interactions”, Soft Matter 20, 9104 (2024).
[3] S. Buyukdagli, “Unified theory of equilibrium thermodynamics and ion association in aqueous and non-aqueous electrolytes with explicit hard-core size”, J. Chem. Theory Comput. 22, 831 (2026).

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