

Effective charges and virial pressure of concentrated macroion solutions

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Colloids constitute the basic components of many everyday products and are integrated into the fabric of modern society. Understanding their assembly is key for nanotechnological and biotechnological advances. At the single-particle level, colloids commonly possess electric charge. Consequently, the structure to which they conform is strongly influenced by electrostatic interactions. In solution, these interactions are modified by the presence of ions. We have developed a model for computing the corresponding effective electrostatic interactions as well as the osmotic pressure. Our model extends the applicability of Derjaguin–Landau–Verwey–Overbeek theory to dense systems in which many-body effects are crucial. This will allow previously impossible, mesoscale studies of colloidal assembly to be performed analytically or by simulation with implicit ions models.

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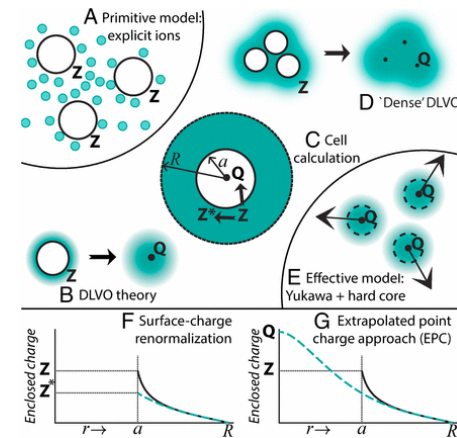


Fig. The various paths (B–D) from the PM (A) of monovalent microions and macroions of valency Z to the effective model (E) where interactions are hard-core Yukawa with effective point charges Q . (F and G) PB cell calculations for the electric field (or charge within radius r) around a macroion following from nonlinear calculations (full line) and the Debye–Hückel fit (dashed line); F illustrates how surface charge renormalization yields a charge Z^* that can be inserted into DLVO theory. In the EPC approach, the effective point charge Q is calculated directly from the extrapolation displayed in G.