An exact method to obtain effective electrostatic interactions from computer simulations: The case of effective charge amplification

Pedro González-Mozuelos, Guillermo Iván Guerrero-García and Mónica Olvera de la Cruz
Department of Materials Science & Engineering, Northwestern University, Evanston, IL, USA

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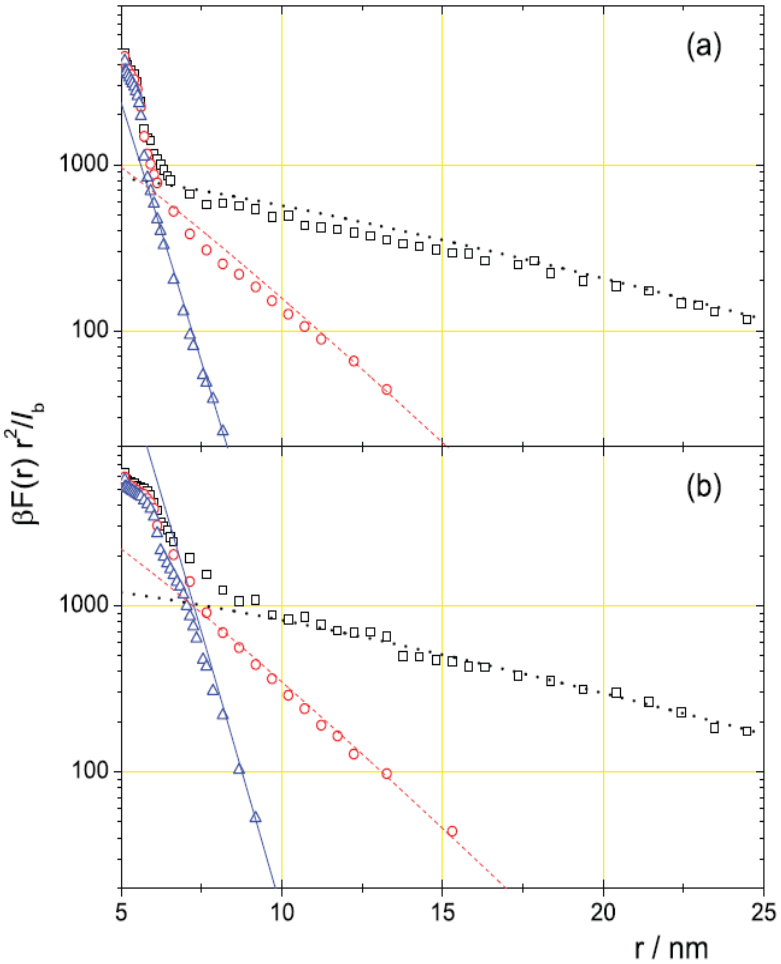

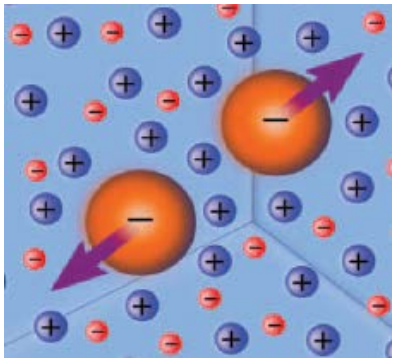

We discuss here an exact method to determine the parameters regulating the screened Coulomb interactions among spherical macroions immersed in a simple electrolyte. This approach provides rigorous definitions for the corresponding screening length, effective permittivity, and renormalized charges, and can be employed for precise and reliable calculations of these parameters within any scheme.
In particular, we introduce a simple procedure for extracting this information from computer simulations.

Figure: *(left) Mean forces between two identical charged nanoparticles (times the square separation distance) immersed in a 1:1 size-asymmetric electrolyte. The nanoparticles have size d_M = 5.1 nm and charge q_M = −90, while the anion size is d_a = 0.3 nm in all instances. In panel (a), the cation size is d_c = 0.5 nm, whereas in panel (b) the cation size is dc = 1.0 nm. In both panels, the following salt concentrations were considered: 0.002 M (squares), 0.02 M (circles), and 0.2 M (triangles). The symbols correspond to MD simulations results (errors are at most of the size of the corresponding symbol), while the lines correspond to the asymptotic Yukawa forces determined in this work.*

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