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On the influence of physical parameters on the properties of the electric double layer modelled by soft potentials. A Monte Carlo study

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Abstract

Grand canonical Monte Carlo results are reported for an electric double layer formed by a planar electrode and spherical ions. The non-electrostatic interactions are the soft interactions approximated by the Lennard-Jones (LJ) potential. In particular, the ion-ion interactions are described by the 12-6 LJ potential, while the ion-electrode interactions are given by the 9-3 potential. The ion charge is located at the centre of a sphere. Ions are immersed in a continuous dielectric medium whose relative permittivity is equal to that of a solvent. The results of simulations for a 1:1 electrolyte and the same ion diameters show that the singlet distribution function of counter-ions has a single high maximum, while that of co-ions has two small maxima. The maxima of counter- and co-ions increase with increasing ion-ion or ion-electrode soft interactions, with decreasing temperature or electrolyte concentration. Analogous changes in the soft interactions, temperature and electrolyte concentration lead to formation at some distance from the negatively charged electrode surface of a negative

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