



"Soft-Matter Seminar"

Coarse-grained simulations of charge, current and flow in heterogeneous media

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Abstract:

The study of complex fluids and heterogeneous materials offers significant challenges because of the wide range of relevant length and time scales involved. Flow in porous media, the equilibrium and kinetic properties of membranes, oil/water mixtures or the electrokinetics (coupled ionic and solvent fluxes) of drops and colloids are examples of situations where the system evolves on scales much larger than molecular ones. I will present a coarse-grained simulation method for complex charged systems. This mesoscopic model couples a hydrodynamic description to a free energy functional accounting for the interactions between solvent(s) and charged solutes. It is implemented in a hybrid lattice-based algorithm, whereby the evolution of the overall mass and momentum is taken care of via a Lattice Boltzmann scheme, whereas the composition and ionic concentrations are updated using the so called link-flux method [1]. I will illustrate the power of this coarse-grained model on several examples involving charged solid-liquid and liquid interfaces [2,3].

[1] F. Capuani, I. Pagonabarraga and D. Frenkel, J. Chem. Phys. 121, 973 (2004)

[2] B. Rotenberg, I. Pagonabarraga and D. Frenkel, Europhys. Lett., 83, 34004 (2008)

[3] B. Rotenberg, I. Pagonabarraga and D. Frenkel, Faraday Discussions (2009)

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