



"Soft-Matter Seminar"

Dr. Joachim Dzubiella

Emmy-Noether-Fellow, TU Garching

Coupling nonpolar and polar solvation free energies in implicit solvent models

Recent studies on the solvation of atomistic and nanoscale solutes indicate that a strong coupling exists between the hydrophobic, dispersion, and electrostatic contributions to the solvation free energy, a facet not considered in current implicit solvent models. We suggest a theoretical formalism which accounts for coupling by minimizing the Gibbs free energy of the solvent with respect to a solvent volume exclusion function. The resulting differential equation is similar to the Laplace-Young equation for the geometrical description of capillary interfaces, but is extended to microscopic scales by explicitly considering curvature corrections as well as dispersion and electrostatic contributions. Unlike existing implicit solvent approaches, the solvent accessible surface is an output of our model. The presented formalism is illustrated on spherically or cylindrically symmetrical systems of neutral or charged solutes on different length scales. The results are in agreement with computer simulations and, most importantly, demonstrate that our method captures the strong sensitivity of solvent expulsion and dewetting to the particular form of the solvent-solute interactions.

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16:00 Uhr

Raum PH 3344

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