



"Soft-Matter Seminar"

„Hydration in discrete water, a cellular automata based approach to obtaining hydration free energies"

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Abstract:

Fast and accurate predictions of hydration free energies are a long standing goal of theoretical biophysics. Despite many years of development, the existing implicit solvent models are still only moderately successful in this area. Here, a discrete water model will be presented, in which some solvent properties are simplified to the extreme, but those most important for molecular hydration: water hydrogen bonding and water-solute electrostatic and dispersion interactions are explicitly taken into account. A solvent distribution around the solute is obtained using a cellular automata type of evolution, and is not dependent on any (pre)defined solvent accessible surface construction. The model is applicable both to small organic compounds and large biomolecules. Apart from providing estimates of hydration free energies, it is also capable of reproducing some nontrivial aspects of protein hydration like dry hydrophobic cavities or isolated, localized water molecules.

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