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Ions without Charges, Hydrogen-Bonds without Hydrogen: Coarse-Grained Models with Short-Range, Anisotropic Interactions

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Water, ions, hydrophilic and hydrophobic moieties are the building blocks of materials and biomolecules. Modeling of the hydrogen-bonded structure of water is particularly challenging for coarse-grained simulations. Nevertheless, reproducing the hydrogen-bonded order of water is necessary not only to reproduce the anomalous thermodynamics, structure and dynamics of liquid water, but also its properties as solvent of ions and hydrophobes, and water-driven interactions. In this talk I will discuss a strategy for the development of coarse-grained models based on short-range anisotropic interactions, and their application for the development of accurate and efficient coarse-grained models of water, solvated ions and DNA, methane and hydrophobic nanoparticles and cavities. These models are 100 to 1000 times computationally more efficient than atomistic models while having quite high fidelity in the description of the structure and -with some caveats- their thermodynamics. I will discuss the level of agreement of the coarse-grained simulations with experimental or atomistic results, and highlight some of their applications.