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Biopolymers in Aqueous Medium: Solvent Forces Explored through Atomistic Dynamics Simulations and Continuum Modeling of Solvent Effects SERGIO A. HASSAN, CMM/DCB/CIT/NIH/U.S.DHHS —

Molecular interactions in solution are modulated by the bulk liquid and by the solvent-induced forces (SIF) originating in the structure of the liquid surrounding the solutes. Because of the difficulty in representing these effects, purely empirical solvation models are commonly used in simulations. Here, a semi-empirical continuum model is presented based on the theory of polar/polarizable liquids, which allows for a derivation of the electrostatic component of the potential. The effects of SIF are still introduced empirically to reproduce interaction energies in amino acids dimers (AAD). The limitations of the model are discussed based on its performance to reproduce structural, dynamic, and thermodynamic properties of peptides and proteins. To reduce the level of empiricism, the molecular origins of the SIF are investigated through dynamics simulations in explicit solvent. The solvent forces on AAD in pure water and NaCl solutions are studied. The reorganization of water and ions due to dimer dissociation is analyzed based on spatial density profiles. The solvent forms a network of high-density peaks consistent with extensive H-bonded water clusters. Long-range structural order develops in the space separating the monomers and contributes to the intermolecular SIF. The ions disrupt this network leading to either a stabilization or destabilization of the dimers. The relevance of these results to quantify SIF in complex solutes en route to a parameter-free continuum model is discussed.

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