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Deconstructing Classical Water Models at Interfaces and in Bulk: Hydrophobic Interactions and Hydrogen Bonding[1]

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Using concepts from perturbation and local molecular field theories of liquids we divide the potential of the SPC/E water model into short and long ranged parts. The short ranged parts define a minimal reference network model that captures very well the structure of the local hydrogen bond network in bulk water while ignoring effects of the remaining long ranged interactions. This deconstruction can provide insight into the different roles that the local hydrogen bond network, dispersion forces, and long ranged dipolar interactions play in determining a variety of solvation and other properties of SPC/E and related classical models of water. We use these short ranged models along with local molecular field theory to quantify the influence of these interactions on the structure of hydrophobic interfaces and the crossover from small to large scale hydration behavior. The implications of our findings for theories of hydrophobicity and possible refinements of classical water models will also be discussed.

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