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Hydrophobic interactions at molecular scale. DUBRAVKO SABO, SAMEER VARMA, SUSAN REMPE, MARCUS MARTIN, Sandia National Laboratories — Structural and thermodynamic properties are investigated for one of the simplest hydrophobic solutes, a hydrogen molecule solvated in liquid water. The structural properties are calculated using different representations of the intermolecular interactions within molecular dynamics, Monte Carlo and ab initio molecular dynamics simulation frameworks. Although structural details differ in the radial distribution functions obtained by different force fields all approaches agree that 16 water molecules coordinate hydrogen. The thermodynamic properties are investigated using Monte Carlo molecular simulation and the quasichemical theory of liquids. Results show that the net hydration free energy arises from a balance between chemical association and molecular packing. Additionally, the results suggest the molecular packing is almost equally driven by unfavorable enthalpic and entropic components.

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