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The Hydrophobic Effect ab initio

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We employ fully quantum-mechanical molecular-dynamics simulations to evaluate the force between two methanes dissolved in water, as a model for hydrophobic association. A stable configuration is found near the methane-methane contact separation, while a shallow second potential minimum occurs for the solvent-separated configuration. The strength and shape of the potential of mean force are in conflict with earlier classical-force-field simulations but agree well with a simple hydrophobic burial model which is based on solubility experiments. Examination of solvent dynamics reveals stable water cages at several specific methane-methane separations.