Potential of mean force of association of hydrophobic particles: dependence on size and temperature

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We carried out molecular dynamics (MD) simulations with AMBER force field for three pairs of dimers (neopentane, bicyclooctane, fullerene-C_{60} molecules) using TIP3P model of water as a solvent. To asses entropy contribution to the Gibbs free energy MD simulations were then run at three temperatures 273K, 323K, and 348K using umbrella-sampling/WHAM method. The stability of dimers is described by potential of mean force (PMF). The shape of PMF curves is characteristic for hydrophobic interactions with a contact minimum, a solvent-separated minimum and a desolvation maximum. The depth and position of the contact minimum for each pair changes with the size of nonpolar particle, consequently the larger molecules shifted to larger distances. Additionally, the contribution of Lennard-Jones potential to PMF increases simultaneously with increase of the particles' size. It is shown, the hydrophobic surface between two interacting particles, entrapes water molecules. We observed, that the contact minima on PMF curves increase with temperature. This means that the association entropy is positive. The dimensionless PMF curves showed low tendency (near contact minima area) of temperature effect, the association entropy is low.