

Origin of hydrophobicity

Hydrophobicity is one of the most important phenomena in science, but its origin at the fundamental level remains unclear. We are focusing on molecular mechanisms in aqueous solutions of small apolar solutes giving rise to the key elements of the hydrophobic effect, such as the entropy loss during hydration (**3**), the origin of the hydrophobic association (**4**), and the manifestation of the structural order around solutes (**5**). Using Monte Carlo simulations together with the classical force-fields we observed the occurrence of strongly correlated exchange of hydrogen bonds between water molecules in the vicinity of hydrophobic solutes. We found that correlations in interaction between water molecules arise as a consequence of reduction of fluctuations in the electrostatic field, which is due to the presence of the inert hydrophobic molecule. In our recent study based on the vibrational spectroscopy and *ab-initio* molecular dynamics simulations (submitted) we have shown that strength of water-water hydrogen bonds in the immediate vicinity of the purely hydrophobic solutes (methane, ethane, krypton, and xenon) is enhanced which emerges as the most fundamental trigger of the hydrophobic effect.

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