

The physical origin of hydrophobicity - Joze Grdadolnik - National Institute of Chemistry, Slovenia**Joze Grdadolnik, Franci Merzel and Franc Avbelj**

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Abstract

Hydrophobicity plays an important role in numerous physicochemical processes, from the process of dissolution in water to protein folding, but its origin at the fundamental level is still unclear. The classical view of hydrophobic hydration is that in the presence of a hydrophobic solute, water forms transient microscopic 'icebergs' arising from strengthened water hydrogen bonding, yet there is no experimental evidence for enhanced hydrogen bonding and/or 'icebergs' in such solutions. We have used the redshifts and line-shapes of the isotopically decoupled infrared O-D stretching mode of small, purely hydrophobic solutes (methane, ethane, krypton, xenon) in water to study hydrophobicity at the most fundamental level. We will present the first unequivocal and model-free experimental proof for the presence of strengthened water hydrogen bonds near four hydrophobic solutes, matching those in ice and clathrates. The water molecules involved in the enhanced hydrogen bonds display extensive structural ordering resembling that in clathrates. The number of ice-like hydrogen bonds is 10 to 15 per methane molecule.

Ab initio molecular dynamics simulations have confirmed that water molecules in the vicinity of methane form stronger, more numerous and more tetrahedrally oriented hydrogen bonds than those in bulk water, and that their mobility is restricted. We demonstrate the absence of intercalating water molecules that cause the electrostatic screening (shielding) of hydrogen bonds in bulk water as the critical element for the enhanced hydrogen bonding around a hydrophobic solute. Our results confirm the classical view of hydrophobic hydration.