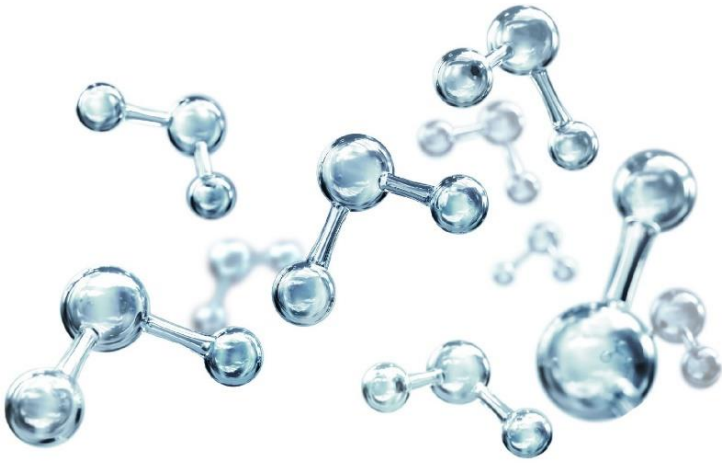
Seminar

CMWS Centre for Molecular Water Science

8th of May 2025
12:00 h (CEST)

Zoom Virtual Meeting:

https://tuhh.zoom.us/j/82631283465
Meeting-ID: 826 3128 3465
Password: 978444



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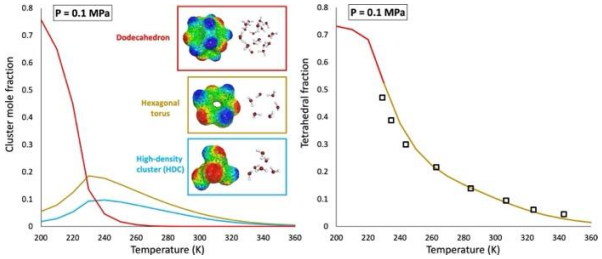
The Shape of Water - how cluster formation explains water's anomalous properties and the hydrophobic effect

Water, essential to life on Earth, has many anomalous properties, that are not yet fully understood. We used density functional theory, the COSMO-RS implicit solvent model and statistical thermodynamics to calculate the dynamic equilibrium of formation of water clusters in water [1]. Clusters of certain shape are predicted to be thermodynamically stable at ambient down to supercooled conditions and their presence almost quantitatively explains water's anomalous properties as a function of temperature and pressure. The dodecahedron is the dominant cluster below ~235 K and below ~150 MPa and forms a miscibility gap with water below a critical point at ~230 K. The hexagonal torus is the dominant cluster above ~235 K and below ~75 MPa. Both the dodecahedron and the torus are low-density clusters, and their presence explains the density maximum of pure water at 277 K (+4 °C). The waters in these clusters are tetrahedrally coordinated, their structures are consistent with experimental data and their presence explains the observed tetrahedral fraction as a function of temperature. A significant part of the overall thermodynamic stability comes from the configurational entropy of the hydrogen bond network in the clusters, so dynamic cluster formation and reformation would be observed as fluctuations in the water structure, rather than stable clusters. At pressures above ~100 MPa, many of water's anomalous properties diminish or vanish, which is also the pressure above which high-density water clusters become more stable and prevalent. Our simple unifying 3-cluster theory reproduces water's anomalous properties from supercooled to ambient temperatures and from ambient pressure up to at least 400 MPa, including density anomalies, two-liquid behavior, compressibility, and heat capacity.

The hydrophobic effect is a particular characteristic of water, related to organic molecule solubility in water and protein folding temperature dependency. A unifying molecular scale origin of these observations has been sought for decades. We have found that the same model that explains water's anomalous behavior simultaneously explains the hydrophobic effect [2]. Including water cluster formation predicts the correct thermodynamics of organic molecule solvation in water as well as surfactant self-assembly. Our model provides an intuitive explanation that water as a whole becomes more hydrophobic as temperature decreases, because higher concentrations of clusters favor internal hydrogen bonds, which leads to fewer opportunities for interactions with solutes.



[1] Andersson, M.P. *J. Mol. Liq.* **383**, 122169 (2023). https://doi.org/10.1016/j.molliq.2023.122169
[2] Andersson, M.P. *J. Mol. Liq.* **400**, 124491 (2024). https://doi.org/10.1016/j.molliq.2024.124491