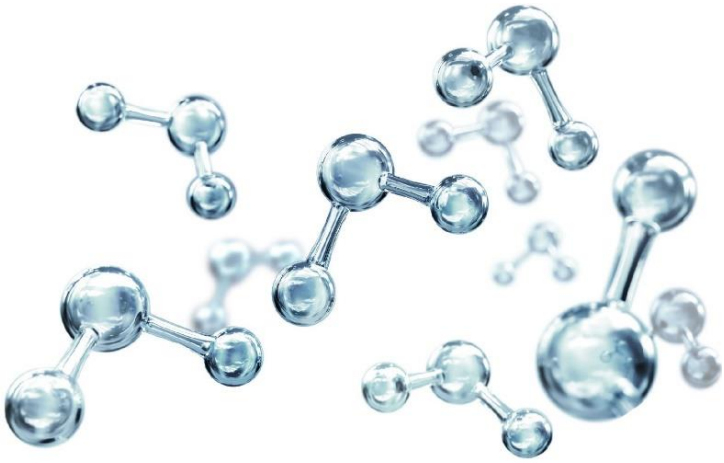
Seminar

CMWS Centre for Molecular Water Science

27th of June 2024
12:00 h (CEST)



Zoom Virtual Meeting:

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

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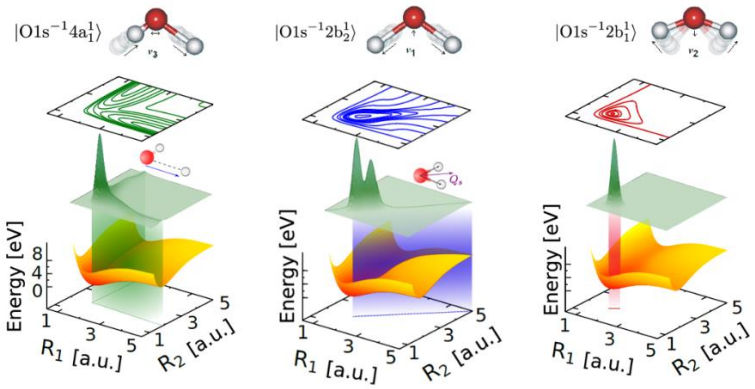
Cuts through the manifold of molecular H2O potential energy surfaces in liquid water at ambient conditions

Liquid water at ambient conditions is ubiquitous in chemistry and biology as well as in technology, energy, and atmospheric processes. Since parts of the phase diagram of water are unsettled - most notably the supercooled liquid homogeneous nucleation region - repercussions thereof on our molecular-level understanding for even the common ambient conditions remain. Breathtaking advances in X-ray–based approaches over the last decade give us now the tools to derive molecular potential energy surfaces as a quantitative view on the molecular manifold within the fluctuating hydrogen bonding network. With selective cuts along the local asymmetric OH bond coordinate and the symmetric normal mode excitations an experimental foundation to benchmark competing molecular-level models of water has been achieved [1].

In this talk, I will present how subnatural line width resonant inelastic X-ray scattering allows to quantify the water molecular potential energy surfaces. In particular, the fluctuating hydrogen bridge bonded network of liquid water at ambient conditions entails a varied ensemble of the underlying constituting H2O molecular moieties. This is mirrored in a manifold of the H2O molecular potentials, ranging from the weak interaction limit to strongly distorted potentials. These will be put into perspective to established parameters, i.e., intermolecular O–H, H–H, and O–O correlation lengths from neutron scattering [2].



[1] S. Eckert et al., Phys. Rev. A 97, 053410 (2018); R. C. Couto et al., Nat. Commun. 8, 14165 (2017); V. Vaz da Cruz et al., Phys. Chem.Chem. Phys. 19, 19573–19589 (2017).
[2] A. Pietzsch et al., Proc. Nat. Acad. Sciences 119, e2118101119 (2022).