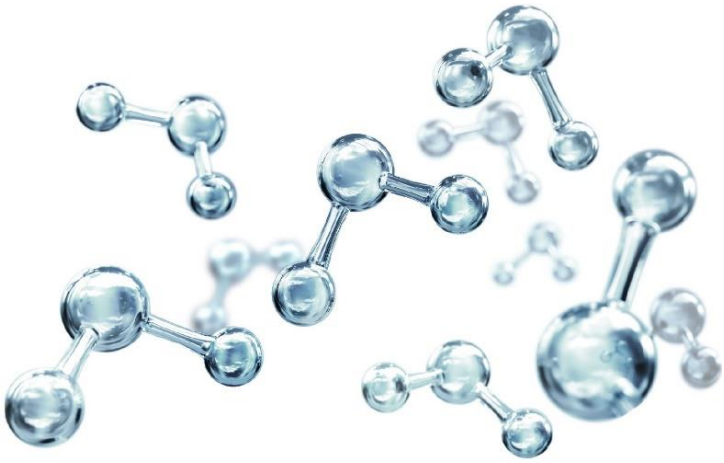
Seminar

CMWS Centre for Molecular Water Science

11th of January 2024
14:00 h

Zoom Virtual Meeting:

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



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Hydration free energy contributions to biological and electrochemical processes

The last decades have seen an explosion of scientific interest in hydrophobic solvation due to its importance for biology, catalysis and environmental science. Recently, we started to realize how important hydrophobicity is also for electrochemical processes. However, understanding and predicting the contributions of solvation and hydrophobicity to the free energy changes during biological and electrochemical processes remains a challenge for both theory and experiments, as it requires dissecting local contributions with high spatial and temporal resolution, as well as understanding how the free energy is tuned by the molecular environment.

In the first part of this seminar,[1,2] I will present a novel approach, “THz-calorimetry”, that accesses solvation entropy and enthalpy changes directly from vibrational spectroscopy observables. THz-calorimetry allows to quantitatively determine solvation entropy and enthalpy with high temporal resolution, down to ps, and to dissect the local contributions from cavity-formation (i.e. hydrophobicity) and attractive solute-water interactions. I will illustrate with a few applications how this knowledge can be used to tune biological processes. In the second part,[3,4] I will discuss some of the additional complexities that arise when dealing with solvation properties at electrified metal-water interfaces, due to the layering of the electrolyte close to the metal and to the applied voltage. On the one side, I will discuss the shortcut of existing solvation theories and the main concepts that must be introduced for electrochemical interfaces. On the other side, I will show examples of how these new complexities open appealing perspective for electrochemical reactions steering, by tuning the hydrophobicity that naturally exists at metal-aqueous interfaces.

(1) S. Pezzotti, F. Sebastiani, E. P van Dam, S. Ramos, V. Conti Nibali, G. Schwaab, M. Havenith, Angew. Chem., Int. Ed. 61, e202203893 (2022); (2) S. Pezzotti, B. Konig, S. Ramos, G. Schwaab, M. Havenith, J. Phys. Chem. Lett. 14, 1556 (2023); (3) A. Serva, M. Salanne, M. Havenith, S. Pezzotti, Proc. Natl. Acad. Sci. 118, e2023867118 (2021); (4) A. Serva, M. Havenith, S. Pezzotti, J. Chem. Phys. 155, 204706 (2021).