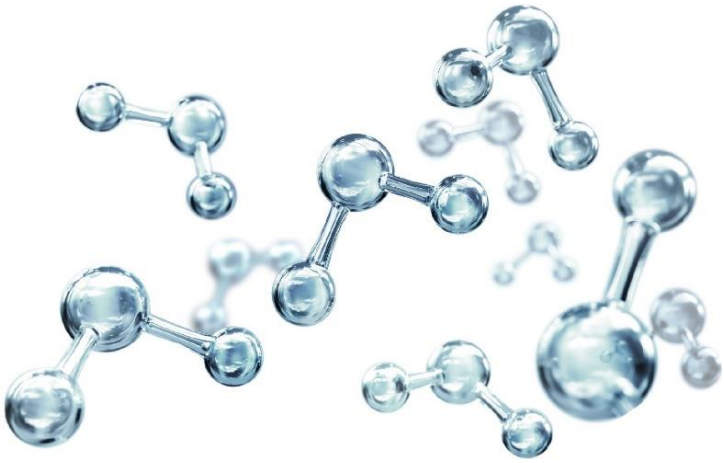
Seminar

CMWS Centre for Molecular Water Science

30th of January 2025
12:00 h (CET)

Zoom Virtual Meeting:

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



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Atomistic modelling of water/solid interfaces

Structures and processes at water/solid interfaces play an important technological role in a wide range of areas such as electrochemical energy conversion and storage, photoconversion, sensors, and corrosion, just to name a few. Still, our understanding of the structure of water/solid interfaces is still limited. This is due to the fact that the liquid nature of water in principle requires to perform statistical averages which can numerically be rather time consuming [1]. Furthermore, for many water/solid interfaces the explicit consideration of the electronic degrees of freedom is necessary [2], in particular as far as electrochemical systems are concerned. This makes the atomistic modelling of water/solid interfaces very demanding. Still there has been recent progress with respect to the atomistic modelling of water/metal interfaces based on ab initio molecular dynamics (AIMD) simulations [2].

In this presentation, I will particularly focus on AIMD studies of water/metal interfaces but also touch water/oxide interfaces. There will be a particular focus on the structure of the water molecules directly at the solid surface. As far as electrochemical water/solid interfaces are concerned, there is a crucial control parameter that needs to be taken into account, the electrode potential [3] which adds further complexity to the modelling. I will also illustrate how simulations of water/solid interfaces under potential control can be performed.

[1] F. Domínguez-Flores, T. Kiljunen, A. Groß, S. Sakong, and M.M. Melander, J. Chem. Phys. **161**, 044705 (2024).
[2] S. Sakong and A. Groß, *Chem. Rev.* **122**, 10746-10776 (2022).
[3] A. Groß, J. Phys. *Chem. C* **126**, 11439-11446 (2022).