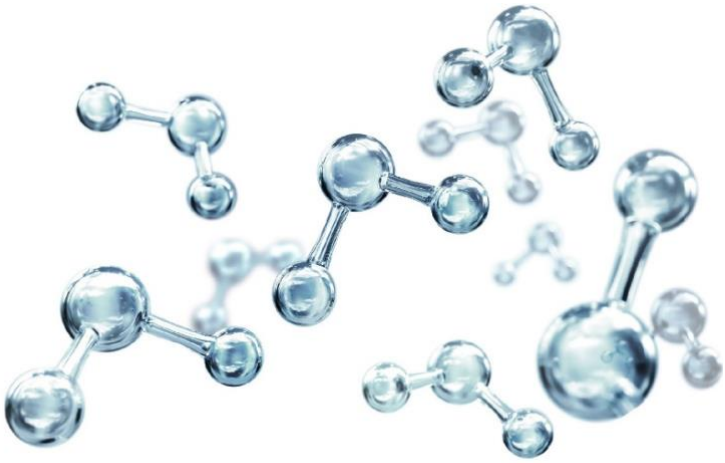
Seminar

CMWS Centre for Molecular Water Science

17th of November 2022
12:00 h

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



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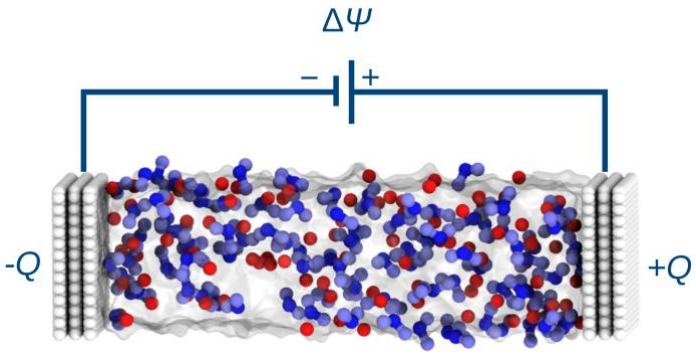
Atomistic simulations of the electrochemical solid/liquid interface



Topics relevant to the energy transition such as corrosion, energy storage and power generation are closely related to processes at the electrochemical interface. However, the electrified solid-liquid interface represents a rather challenging system for fundamental simulation approaches such as ab initio calculations or molecular dynamics. In this talk, I will present the results of an ab initio study of the fundamental corrosion processes on magnesium [1] and explain how promising corrosion modulators can be identified using machine learning to influence these processes [2,3]. Importantly, ab initio simulations typically cannot account for the entire electrical double layer, so more efficient approaches must be used. I will present results on double layer capacitance from classical molecular dynamics simulations for curved electrodes [4] using our recently implemented electrochemistry package in LAMMPS [5]. In addition, if time allows, I will show preliminary results on redox reactions in a pseudocapacitor using ab initio molecular dynamics at constant potential, which is a challenge that cannot be overcome using classical molecular dynamics. Finally, I conclude that it would be beneficial to link these approaches in a multiscale sense to create a better understanding of such complex systems where processes at all scales play an important role.

References

[1] Würger, T., Feiler, C., Vonbun-Feldbauer, G.B. et al. A first-principles analysis of the charge transfer in magnesium corrosion. Sci Rep 10, 15006 (2020). https://doi.org/10.1038/s41598-020-71694-4

[2] Würger, T., Mei, D., Vaghefinazari, B. et al. Exploring structure-property relationships in magnesium dissolution modulators. npj Mater Degrad 5, 2 (2021). https://doi.org/10.1038/s41529-020-00148-z

[3] Würger, T., Wang, L., Snihirova, D. et al. Data-Driven Selection of Electrolyte Additives for Aqueous Magnesium Batteries. J Mater Chem A 10, 21672–21682 (2022). https://doi.org/10.1039/d2ta04538a

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[5] Ahrens-Iwers, L.J.V, Janssen, M., Tee, S.R. et al. ELECTRODE: An electrochemistry package for atomistic simulations. J Chem Phys 157, 084801 (2022). https://doi.org/10.1063/5.0099239