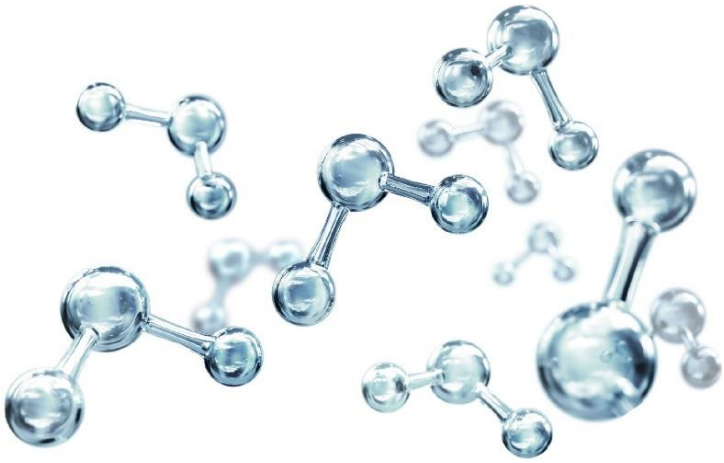
Seminar

CMWS Centre for Molecular Water Science

21th of April 2022
12:00 h

Zoom Virtual Meeting:

https://desy.zoom.us/j/84703564086
Meeting-ID: 847 0356 4086
Password: 570173



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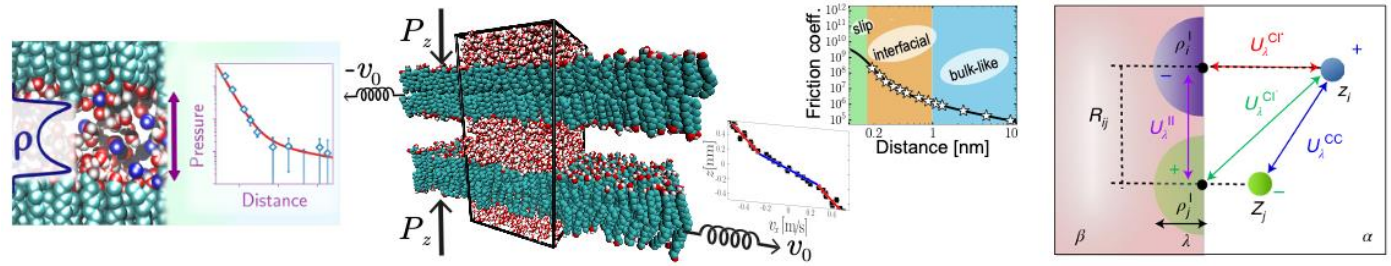
From interfaces to confinement – water's peculiar behavior on the nanoscale

Water shows a broad range of intriguing effects at interfaces that are strongly linked to its biological and technological relevance. In this talk, I will show how we can exploit atomistic simulations in order to construct *effective* yet *predictive* models as a powerful tool for biological and technical applications such as filtration, catalysis, etc. I will briefly introduce the emergence of hydration forces that ultimately stabilize biological systems [1]. In particular, I will focus on hydration friction and water transport in soft nano-confinement [2].

Water's intricate structure at interfaces leads to the emergence of dielectric effects [3] that in confinement lead to a strong modification of electrostatic interactions [4]. I will speculate that specific knowledge of such interactions might open new possibilities for energy storage as well as (electro-) chemistry [5].



References

[1] A. Schlaich, B. Kowalik, M. Kanduč, E. Schneck, and R. R. Netz, *Physical Mechanisms of the Interaction between Lipid Membranes in the Aqueous Environment*, Physica A **418**, 105 (2015). [2] A. Schlaich, J. Kappler, and R. R. Netz, *Hydration Friction in Nanoconfinement: From Bulk via Interfacial to Dry Friction*, Nano Lett. **17**, 5969 (2017). [3] A. Schlaich, E. W. Knapp, and R. R. Netz, *Water Dielectric Effects in Planar Confinement*, Phys. Rev. Lett. **117**, 048001 (2016). [4] A. Schlaich, A. P. dos Santos, and R. R. Netz, *Simulations of Nanoseparated Charged Surfaces Reveal Charge-Induced Water Reorientation and Nonadditivity of Hydration and Mean-Field Electrostatic Repulsion*, Langmuir **35**, 551 (2019). [5] A. Schlaich, D. Jin, L. Bocquet, and B. Coasne, *Electronic Screening Using a Virtual Thomas–Fermi Fluid for Predicting Wetting and Phase Transitions of Ionic Liquids at Metal Surfaces*, Nat. Mater. 1 (2021).