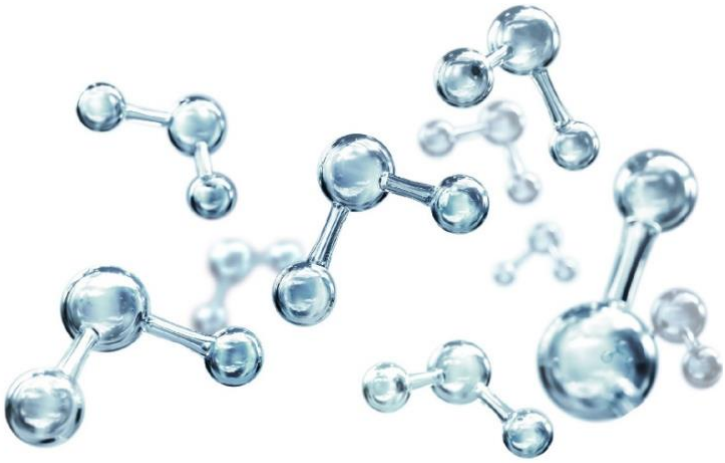
Seminar

CMWS Centre for Molecular Water Science

12th of January 2023
12:00 h

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



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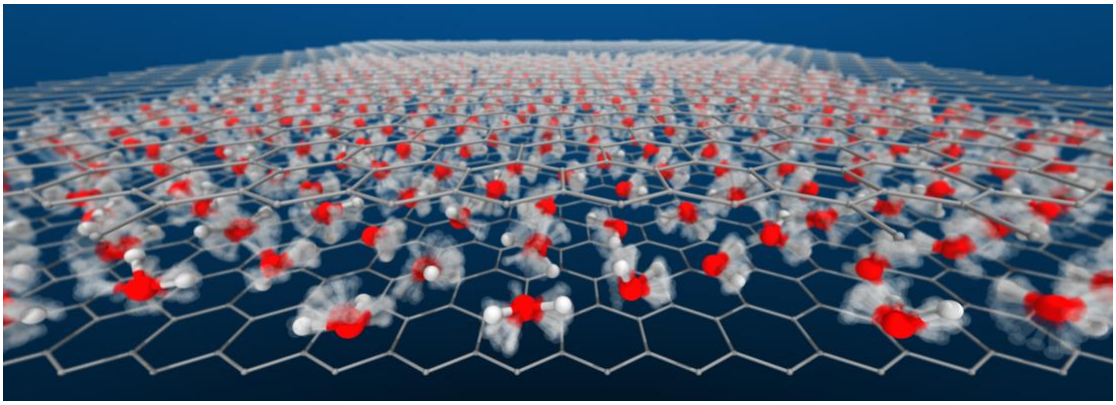
Understanding complex aqueous systems with machine learning

Simulation techniques based on accurate and efficient representations of potential energy surfaces are urgently needed for the understanding of complex systems such as solid-liquid interfaces. In this talk, we present our recent methodological advances for machine learning potentials enabling the efficient development and validation of models for complex aqueous systems.[1,2] Building on the seminal work by Behler and Parrinello, we make use of committee models providing accuracy improvements, measures of uncertainty, and strategies for active learning.[1] These features enable the streamlining of the development of new models in an end-to-end framework to tackle complex aqueous systems.[2] Finally, we demonstrate the capability of these approaches for providing insight into the water flow in single-wall nanotubes[3] as well as the complex phase behaviour of mono-layer confined water[4].



References

[1] C. Schran, K. Brezina, O. Marsalek, J. Chem. Phys., 2020, 153, 104105

[2] C. Schran, F. L. Thiemann, P. Rowe, E. A. Müller, O. Marsalek, A. Michaelides, Proc. Nat. Acad. Sci., 2021, 118 (38), e2110077118

[3] F. L. Thiemann, C. Schran, P. Rowe, E. A. Müller, A. Michaelides, ACS Nano, 2022, 16, 7, 10775–10782

[4] Kapil, C. Schran, A. Zen, J. Chen, C. J. Pickard, A. Michaelides, Nature, 2022, 609, 512–516