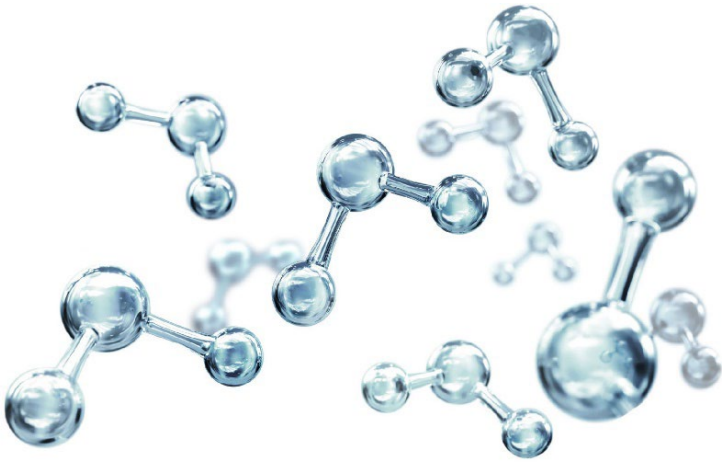
Seminar

CMWS Centre for Molecular Water Science

19th of October 2023
14:00 h (CEST)

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



Mariana Rossi

Max Planck Institute for the Structure and Dynamics of Matter
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Simulating atomic and electronic properties of water with *ab initio* accuracy at larger scales

In this talk, I will discuss first-principles atomistic simulation techniques capable of capturing the atomic structure and dynamics, as well as the electronic structure of water-based systems at larger scales. I will give special focus to the importance of nuclear quantum effects on water dissociation events at defects [1,2] and charged metallic surfaces, and to new techniques for the computation of vibrational fingerprints of water interfaces. I will finish with the discussion of machine-learning methods that allow the computation of electronic properties and responses of water in several phases at larger system sizes [3,4].

[1] Y. Litman, et al, *J. Chem. Phys.* **148**, 102320 (2018)
[2] K. Fidanyan, J. Liu, M. Rossi, *J. Chem. Phys.* **158**, 094707 (2023)
[3] A. Lewis, et al., *J. Chem. Theory Comput.* **17**, 7203–7214 (2021)
[4] A. Lewis, P. Lazzaroni, M. Rossi, *J. Chem. Phys.* **159**, 014103 (2023)