CFEL SCIENCE

SEMINAR

16th October 2024 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Weakly Bound Materials: Competing Energy Scales, Quantum Effects, and Machine Learning

Weakly bonded interfaces, commonly encountered in hybrid organic-inorganic architectures, give rise to a rich variety of nuclear motion and tunable nuclear structure that is tightly connected to diverse electronic properties in these systems. In this contribution, I will discuss how we push the limits of density-functional theory and different ab initio techniques that capture nuclear motion to unravel the properties of realistic interfaces. I will give an overview of simulation methods that are applicable for large system sizes and that can capture the quantum nature of nuclei in anharmonic potential energy landscapes [1]. I will discuss how they can be connected to first-principles electronic structure and machine-learning approaches [2,3]. Applications where the quantum nature of the nuclei become indispensable to assess structural and electronic properties of 2D materials and interfaces will be shown and discussed [4], as well as how these can be characterised by the simulation of experimentally observable quantities like tunneling rate constants and advanced vibrational spectroscopy [5,6].

[1] M. Rossi, *J. Chem. Phys.* **154**, 170902 (2021).

[2] A. M. Lewis, A. Grisafi, M. Ceriotti, and M. Rossi, *J. Chem. Theory Comput.* **17**, 7203 (2021).

[3] A. M. Lewis, P. Lazzaroni, and M. Rossi, *J. Chem. Phys.* **159**, 014103 (2023).

[4] A. Schobert *et al.*, *SciPost Phys.* **16**, 046 (2024).

[5] Y. Litman *et al.*, *J. Chem. Phys.* **156**, 194106 (2022).

[6] Y. Litman, F. Bonafé, A. Akkoush, H. Appel, M. Rossi, *J. Phys. Chem. Lett.* **14**, 6850 (2023).

Host: Robin Santra – CFEL-DESY Theory Division