www.physik.uni-stuttgart.de/aktuelles/kolloquium

Stuttgarter Physikalisches Kolloquium

Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme
Fachbereich Physik, Universität Stuttgart

Ansprechpartner: Andreas Schnyder
E-Mail: A.Schnyder@fkf.mpg.de
Telefon: 0711 689-1553

Login data will be announced by e-mail and on the colloquium webpage.

Dienstag, 2. Februar 2021 | **16.15 Uhr** | **Online-Vortrag**

Stuttgarter Max-Planck-Institute, Heisenbergstraße 1, 70569 Stuttgart-Büsnau

Unraveling structural and dynamical properties of (quantum) nuclei in diverse materials

Mariana Rossi
MPI for the Structure and Dynamics of Matter, Hamburg

Abstract

In weakly bonded systems, the nuclear fluctuations induced by temperature can completely change the structure, the thermodynamic equilibrium, and also the electronic structure of materials. In addition, given the ubiquitous presence of light nuclei in organic materials, not only the electrons but also the nuclear fluctuations must be treated within the first principles of quantum mechanics.
In this talk, I will show how we achieve an all-atom, all-electron quantum description of these systems by developing methodology and tools that allow joining density-functional theory calculations to path integral methods. I will show situations, involving organic/inorganic interfaces, where we have solved questions related to a pronounced temperature dependence of electronic properties and charge transfer, as well as apparently contradictory observations in hydrogen transfer reactions. None of this would be possible if the atomic structure of the systems was unknown or incorrect. I will show how we navigate the structure space of weakly bonded interfaces and molecular solids through exhaustive ab initio structure searches and the simulation of structure-sensitive spectroscopic techniques, couple to machine-learning methods to bridge length scales.