

Theoriekolloquium

Am **22. April 2021 um 14.15 Uhr** hält

Frau Dr. Mariana Rossi (Hamburg)

einen Vortrag mit dem Titel

**Simulating weakly-bonded interfaces at finite temperatures with
quantum mechanics for electrons and nuclei**

Atomistic simulations based on the first-principles of quantum mechanics can nowadays reach unprecedented length and time scales. When dealing with weakly bonded systems, new methodologies that allow the treatment of electrons and nuclei as quantum particles become indispensable. I will give an overview of simulation methods that are applicable for large system sizes and that can capture the quantum nature of electrons and nuclei. Applications where the quantum nature of the nuclei become indispensable to assess structural and electronic properties of interfaces will be shown and discussed, as well as how these can be characterised by the simulation of experimentally observable response properties of these systems.

Interessierte sind herzlich eingeladen.

gez. Prof. Dr. Caterina Cocchi