Welcome Seminar

7 Novembre 2024 - h15:00
Aula A

Dr. Emiliano Poli
Ricercatore a tempo determinato di tipo A

Dipartimento di Scienze Chimiche
Università degli studi di Padova

Navigating Complex Boundaries: Challenges in Ab Initio Simulations of Extended Heterogeneous Interfaces.

Interfacial systems are pivotal in numerous technological and biological processes of interest, from protein–water interactions to electronic re-hybridization at metal–organic boundaries. Investigating these systems at the molecular level presents unique challenges for both experimental methods and molecular simulations. In molecular simulations specifically, these challenges range from scaling issues in ab initio calculations to the transferability of empirical force fields in classical simulations.

In this talk, I will discuss several theoretical methods and approximations (such as Linear Scaling DFT, Machine Learned Force Fields and others) that can be employed to address the complexity of heterogeneous interfaces and describe their behavior with ab initio–level precision. To show the effectiveness of these approaches, I will present simulation results for three distinct systems of interest: water/oil interfaces as models for water–protein interactions; metal–organic interfaces aimed at promoting itinerant magnetism; and methane cracking on iron nanoparticles for turquoise hydrogen production.

Finally, I will conclude by discussing potential future developments in simulating electrode interfaces under operando conditions and the work I am undertaking in the group of Prof. Stefano Corni in Padova.

Il Direttore del Dipartimento - Prof. Stefano Mammi