

SEMINAR ANNOUNCEMENT

WEDNESDAY, 29.01.2014
2.15 PM S.T. IN NC 03/399

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"Water interfaces: structure and vibrational spectroscopy from DFT- based MD simulations"

Abstract: Water properties at the interface can be quite different from bulk properties and have been central to several recent investigations. In this seminar I will present an overview of our computational approach to understand liquids properties at the interface including atomistic and electronic structure details. In particular I will show how Density Functional Theory-based molecular dynamics simulations (DFT-MD) of solid/water and water/vapor interfaces can provide a microscopic interpretation of recent experimental results from surface sensitive Vibrational Sum Frequency Generation spectroscopy (VSFG). Organization of water at the interface with oxides including silica and alumina will be discussed. The interfacial hydrogen bond network is investigated in details and is related to the chemistry of the oxide surfaces. In addition I will also present some results for the water/vapor interface, where a full ab initio approach has been applied for the first time to the calculation of the VSFG response function.

Interested persons are cordially invited to attend!