Ab initio molecular dynamics simulations of alumina oxide/water interfaces

GAIGEOT Marie-Pierre; CIMAS Álvaro

CNRS LAMBE, Université Paris-Saclay, Univ Évry, 91025 Évry-Courcouronnes, France

alvaro.cimas@univ-evry.fr

The surfaces and interfaces of metal oxides play an important role in many natural and technological processes such as mineral dissolution, adsorption/desorption reactions, pollutant transport in groundwater, corrosion, and heterogeneous catalysis. In all these processes the structure of the water at the interface with the oxide is a key factor. This is what we investigate with DFT-MD simulations (DFT-based Molecular Dynamics).

We will review our works on a-alumina oxide Al2O3/liquid water interfaces, where we unravel the intertwined structural arrangement of surface and liquid water at the interface. Chemical reactivity is highly dependent on surface structure and speciation at the interface with the solvent, therefore the pre-requisite knowledge of the following points: type of surface, surface sites protonation state (O, OH, OH2), water molecules organization due to the presence of the solid, water and surface site orientations and hydrogen bonding networks. Of particular interest is the comprehension of the H-Bond network formed between the surface aluminols and interfacial water molecules, in terms of which surface chemical types are involved in the network, and in terms of strength of H-Bonds. Also of importance is the relationship between interfacial structures and vibrational signatures. These signatures are calculated from the DFT- MD trajectories (SFG, Sum Frequency Generation) and are compared to experiments.

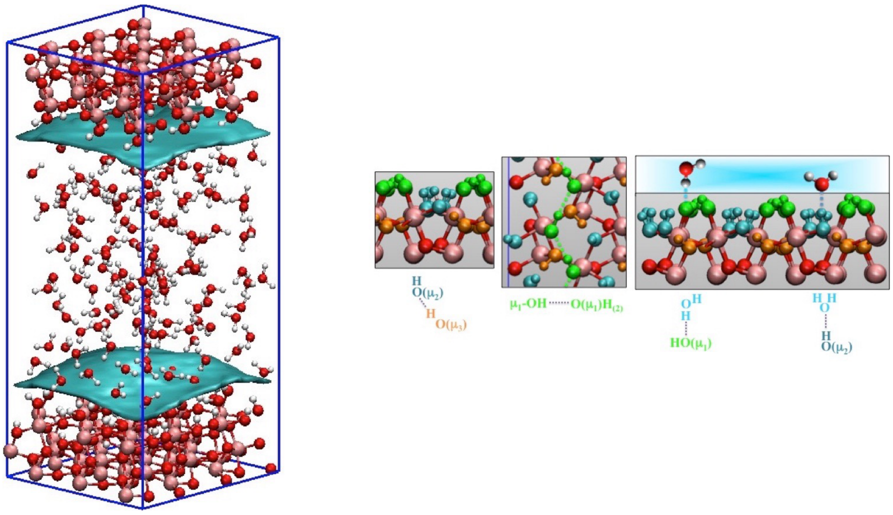

Figure 1. Simulation box (left) and schematic representation of the hydrogen bonding at the interface (right).

KEYWORDS: oxide/water interfaces, ab initio DFT-MD, SFG.