Ab initio molecular dynamics simulations of catalytic alumina oxide/water interfaces

A. CIMAS[1], L. POTIER[1], C. KALAI[1], MARIE-PIERRE GAIGEOT[1]

[1] LAMBE UMR8587, Laboratoire Analyse et Modélisation pour la Biologie et l'Environnement, Université d'Evry val d'Essonne, Blvd F. Mitterrand, Bat Maupertuis, 91025 EVRY, 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, heterogeneous catalysis. Our interest is mainly in this latest domain, and in order to help industries improve the efficiency of some catalytic processes, one needs a detailed knowledge of the interface at the atomic level in terms of interfacial structure and surface termination.

We present DFT-MD simulations of the (0001) and (1$\underline{1}$02) alumina oxide/liquid water interfaces, and unravel the structural arrangement of surface and liquid water at the interface. 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. This will be related to the catalytic activity of the interface. Also of importance is the relationship between interfacial structures and vibrational signatures. These signatures are calculated from the DFT-MD trajectories (IR & SFG in particular) and can be compared to experiments. Simulations including the presence of the Co^{2+} ion at these interfaces, of relevance for catalysis, will also be presented.

The work presented here is part of the ANR SLIMCAT funding, "Stimuler le Renouveau Industriel".