MAR17-2016-000758

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Water at silica/liquid water interfaces investigated by DFT-MD simulations

MARIE-PIERRE GAIGEOT[1], LAMBE UMR8587 Universite d'Evry val d'Essonne

This talk is dedicated to probing the microscopic structural organization of water at silica/liquid water interfaces including electrolytes by first principles DFT-based molecular dynamics simulations (DFT-MD). We will present our very recent DFT-MD simulations of electrolytic (KCl, NaCl, NaI) silica/liquid water interfaces in order to unravel the intertwined structural properties of water and electrolytes at the crystalline quartz/liquid water and amorphous silica/liquid water interfaces. DFT-MD simulations provide direct knowledge of the structural organization of water and the H-Bond network formed between the water molecules within the different water layers above the silica surface. One can furthermore extract vibrational signatures of the water molecules within the interfacial layers from the DFT-MD simulations, especially non-linear SFG (Sum Frequency generation) signatures that are active at solid/liquid interfaces. The strength of the simulated spectra is that a detailed analysis of the signatures in terms of the water/water H-Bond networks formed within the interfacial water layers and in terms of the water/silica or water/electrolytes H-Bond networks can be given. Comparisons of SFG spectra between quartz/water/electrolytes and amorphous silica/water/electrolytes interfaces allow us to definitely conclude on how the structural arrangements of liquid water at these electrolytic interfaces modulate the final spectroscopic signatures.

[1]Invited speaker