SFG spectroscopy of Silica/water interfaces by DFT-MD simulations

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We will present our very recent DFT-MD simulations of electrolytic silica/water interfaces in order to unravel the structural properties of electrolytes at the crystalline quartz/liquid water interface and at the amorphous silica/liquid water interface, including pH effects, and how water and surface both modulate each other response to the presence of electrolytes.

The theoretical method employed to calculate SFG spectra from DFT-MD simualtions is presented. Our strength is in the detailed analyses and assignments of the non-linear SFG spectral signatures based on the detailed knowledge of the interfacial structural organisation.

Our work clearly demonstrates how the structural arrangements of liquid water and electrolytes at silica/water interfaces modulate the final spectroscopic signatures, providing guidelines and marker-bands to be used by experimentalists.