DE LA RECHERCHE À L'INDUSTRIE

Séminaire

Mardi 21 octobre 2014 à 10h30

Salle de réunion du SRMP – Bâtiment 520 - Pièce 109

Microscopic characterization of the fluorite/ water interface from theory and experiments

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The crystal growth and dissolution processes of fluorite (CaF_2) crystals have attracted much attention due to the importance in the industrial, environmental, and medical applications. While previous studies clarified nanoscale processes at the fluorite–water interface, atomic scale origins of the processes have yet to be understood. In this study, we combine Density Functional Theory based molecular dynamics simulation and interface selective spectroscopy in order to investigate atomic-scale structure at the fluorite–water interface as function of pH. We probe for the first time the absolute orientation of the water molecules at the interface and provide a microscopic interpretation for the vibrational spectroscopic signal. Under basic conditions the experimental spectra can be explained by a substitution of F by HO at the interface. Moreover under acidic condition a microscopic model for the charged interface is provided.

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