

The interfacial layer properties in nanoconfinement: an experimental and modelling approach

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The experimental characterization of the interfacial layer (IL) at the surface of silica nanoconfinement filled with water and ions is a scientific challenge but is of great interest to understand the specific geochemical processes occurring into the nanoporosity of clay, mineral and biomineral phases and alteration layers. Indeed, the strong interactions between water molecules and pore surfaces modify the water structure and slow down its dynamics from nanoscale to macro-scale. Also, the presence of solvated ions and the ions adsorbed on the nanopores surface modify the electrostatic interactions in the system and thus the ions energy landscape (IEL).

To determine the IEL modification into the IL, we propose an original approach using model systems consisting in parallel and plane silica surfaces spaced of 3 and 5 nm (nanochannels) filled with electrolytes containing cations having various kosmotrope properties. These nanochannels were characterized using hard X-Ray reflectivity (27 keV at ESRF) during their filling with XCl_2 solutions at 1 M ($X=Mg$, Ca and Mg). From X-ray reflectivity (XRR) curves, the electron density profiles were extracted directly by inverse Fourier transform. In parallel, ions and water distribution in nanochannels were simulated by atomistic modelling. The experimental results show that the nanochannels filling are incomplete depending on the electrolyte used. A local hydrated salt species precipitation in nanochannels due to an ions supersaturation in IL determined from atomistic modelling coupled to a slow down of water/ions transport into the IL may explained this result. This open new perspective to explain the formation of metastable phases in nanoconfinement.

