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Investigating the interfacial solvation properties of the magnesium oxide by operando soft X-ray absorption spectroscopy at ambient pressure

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Interfaces between water and materials are ubiquitous and are crucial in materials sciences and in biology, where investigating the interaction of water with the surface under ambient conditions is key to shedding light on the main processes occurring at the interface. Magnesium oxide is a popular model system to study the metal oxide-water interface, where, for sufficient water loadings, theoretical models have suggested that re-constructed surfaces involving hydrated Mg(II) metal ions may be energetically favored. In this presentation, our group's recent efforts to apply an innovative approach using ambient pressure operando near edge X-ray near structure spectroscopy (AP-NEXAFS) to study the chemical processes occurring at the interphase will be summarized. In particular, by combining experimental and theoretical surface-selective ambient pressure X-ray absorption spectroscopy with multivariate curve resolution and molecular dynamics, we evidence in real time the occurrence of Mg²⁺ solvation at the interphase between MgO and solvating media such as water and methanol. Further, we show that the Mg²⁺ surface ions undergo a reversible solvation process, we prove the dissolution/redeposition of the Mg(II) ions belonging to the MgO surface and demonstrate the formation of octahedral intermediate solvated species. The unique surface, electronic, and structural sensitivity of the developed technique may be beneficial to access often elusive properties of low-Z metal ion intermediates involved in interfacial processes of chemical and biological interest.

if "Other", please specify:

I apply for a travel grant

No

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