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**Solvation of ions investigated by DFT-MD simulations: from gas phase to oxide/liquid water interfaces**

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We investigate the solvation of ions by means of DFT-based molecular dynamics simulations (DFT-MD): ions solvated in clusters and ions solvated at solid oxide/liquid water interfaces. DFT-MD simulations provide a detailed knowledge of the solvation structural properties at finite temperature, and dynamical anharmonic vibrational spectra extracted from DFT-MD are used to detail the relationships between vibrational features and structures. We present recent results for ionic clusters, i.e. solvation of  $\text{Li}^+$  by water molecules in  $\text{Li}^+(\text{H}_2\text{O})_{3,4}$ , including dynamical anharmonic vibrational spectra calculations and comparisons to IR-PD (InfraRed Pre-Dissociation) experiments at different temperatures, also including the dynamical formation of these clusters as it occurs in the experiments and the understanding of how high energy conformers can be formed and probed in these experiments. We also present solvation of electrolytes at the quartz/liquid water interfaces. Here also, not only do we use DFT-MD in order to unravel the structure of these electrolytes at the interface between the oxide and liquid water but we also extract dynamical vibrational spectra to be compared to SFG (Sum Frequency Generation) experiments. With this comparison we aim at a detailed description of the interfacial structure and its related vibrational signatures.

These works have been done in collaboration with Prof J.M. Lisy (USA), Prof M. Sprik (UK), Prof M. Sulpizi (Germany), Dr V. Brites, and M. Pfeiffer.