Probing molecular processes at water-insulator interfaces

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Surface science techniques, and particularly high-resolution Scanning Probe Microscopy (SPM) approaches, now offer unprecedented levels of understanding and control of solid/vacuum interfaces. By contrast, the physics of liquid/solid interfaces is less developed, although it is often more relevant for real-world applications. It is important in such diverse fields as heterogeneous catalysis, next generation battery technology and corrosion. The solid/liquid interface is also particularly relevant to biological systems, where measurements are made in physiological conditions.

In this work we review our general approach for simulating high resolution scanning probe microscopy for solid-liquid interfaces, but then introduce recent results combining first principles and atomistic simulation approaches to study how water interacts with different insulating surfaces, providing atomic-scale insight into hydration structures [1], dissolution [2] and high-resolution imaging. In particular, we consider the interplay on enthalpy and entropy in 3D imaging of calcite, and then we study the complex reconstruction of the SrTiO$_3$ surface, and how it influences the hydration structure and resulting AFM images.
