Computer simulations of solid-liquid interfaces

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Computer simulations provide simultaneously numerous physical quantities, allowing discussion of the results in their complexity. This is not always the case in experiments, sometimes leading to difficulties in interpretation of the origins of the experimental signals. Thanks to advance of simulation techniques allowing description of the inhomogeneous environment, we will demonstrate how simulation can help in molecular-level understanding of the phenomena occurring at solid-liquid interfaces. Particularly, we have investigated the adsorption of water, ions, and molecules on neutral and charged surfaces, characterized the local viscosity, diffusivity and dielectric properties of water molecules at the interface, and described effect of temperature and pH on the dynamics of ions, including electrokinetic phenomena and determination of zeta potential.

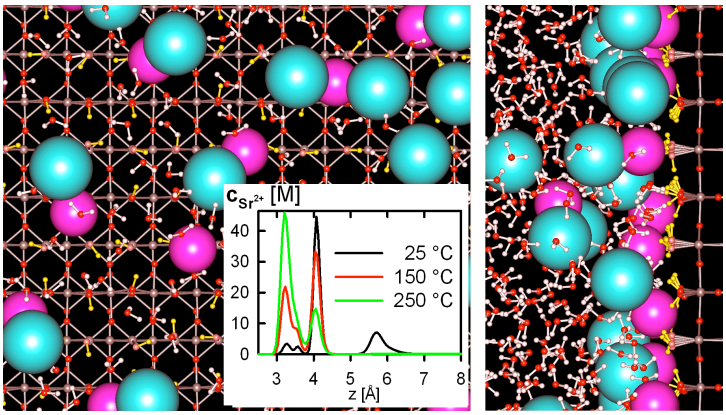

Figure 1: Adsorption of Sr^{2+} ions (pink) and Cl^- (cyan) on the negatively charged (-0.2 C/m^2) rutile surface. The inset shows the temperature dependence of the distribution of cations among inner sphere adsorption sites (distances up to 5 Å) and outer-sphere sites (around 5.8 Å).

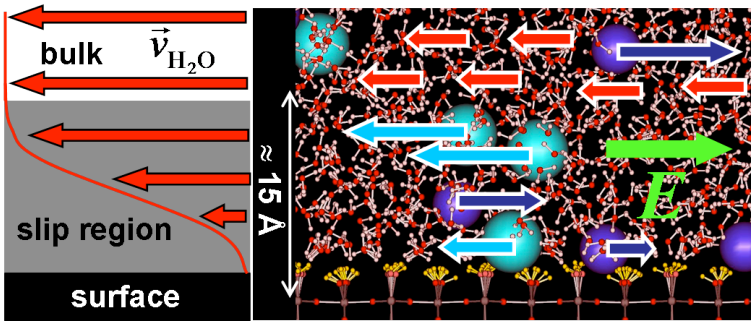

Figure 2: Schematic picture of the molecular origin of electro-osmotic velocity.