Ab initio constant temperature molecular dynamics of liquid-solid interfaces

We will present ab initio molecular dynamics simulations of a variety of solid-liquid interfaces. We calculate the adsorption energy of catechol and HCl on a TiO2(110) surface in the presence and the absence of a water film. We find very large differences in the adsorption energy, which can be qualitatively understood by a simple model that connects the adsorption energy in the presence of water to the adsorption energies in the vacuum. We have also studied the interface of molten LiCl with MgO as a model of the interaction of a solid surface with a strong electrolyte. We find that the solid induces ordering in the liquid which forms layers or alternating positive and negative ions. This is contrary to the Gouy-Chapman model which breaks down completely for the pure ionic, liquid LiCl. We will also present our study of the Pt-water interface in which we show how the liquid structure at the interface is affected by the presence of ions in the liquid and/or charges in the solid surface.