Water at Interfaces: wetting, slip and dielectric effects

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The structural and dynamic properties of the water layer close to anorganic and organic surfaces are relevant for many physico-chemical processes. Examples are protein adsorption or protein stability. Insight can be gained from all-atomistic simulations of water that nowadays reach the experimentally relevant length and time scales. This is demonstrated with a few examples:

i) Hydrophobic (water-repelling) surfaces in contact with water show a pronounced depletion layer with a thickness of a few Angstroms within which the water density is highly reduced.
This layer leads to unusual static and kinetic properties including a finite slip length, which means that water flows with much reduced friction over such surfaces.

ii) The framework for deriving dielectric interfacial profiles from multipole distributions is established and applied to Molecular Dynamics simulations of water at hydrophobic and hydrophilic surfaces.
In conjunction with a modified Poisson-Boltzmann equation, the trend of experimental double layer capacitances and electrokinetic phenomena is well reproduced.