MAR12-2011-020207

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Friction and Hydration Repulsion Between Hydrogen-Bonding Surfaces

ROLAND NETZ, Free University Berlin, Germany

The dynamics and statics of polar surfaces are governed by the hydrogen-bonding network and the interfacial water layer properties. Insight can be gained from all-atomistic simulations with explicit water that reach the experimentally relevant length and time scales. Two connected lines of work will be discussed: 1) On surfaces, the friction coefficient of bound peptides is very low on hydrophobic substrates, which is traced back to the presence of a depletion layer between substrate and water that forms a lubrication layer. Conversely, friction forces on hydrophilic substrates are large. A general friction law is presented and describes the dynamics of hydrogen-bonded matter in the viscous limit. 2) The so-called hydration repulsion between polar surfaces in water is studied using a novel simulation technique that allows to efficiently determine the interaction pressure at constant water chemical potential. The hydration repulsion is shown to be caused by a mixture of water polarization effects and the desorption of interfacial water.