

## Abstract

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[1].

ii) Most proteins readily adsorb on both hydrophobic and hydrophilic surfaces which is a problem when trying to design protein resistant (so called non-fouling) surface coatings. The mechanism behind this universal attraction is not clear but surely involves water.

AFM experiments performed in Munich yield adsorption energies of single protein molecules and point to an extremely high mobility on hydrophobic surfaces. MD simulations suggest that both water structural effects and dispersion interactions between protein and surface contribute to the adsorption energy[2].

iii) The friction coefficient of bound polymers is very low on hydrophobic substrates. This can be traced back to the presence of a vacuum layer between substrate and water, which forms a lubricating cushion on which a polymer can glide[3].

[1] Water slippage versus contact angle: a quasi-universal relationship, D.M. Huang, C. Sendner, D. Horinek, R.R. Netz, and L. Bocquet, *Physical Review Letters* (2008)

[2] Peptide adsorption on a hydrophobic surface results from an interplay of solvation, surface and intrapeptide forces, D. Horinek, A. Serr, M. Geisler, T. Pirzer, U. Slotta, S. Q. Lud, J. A. Garrido, T. Scheibel, T. Hugel, R. R. Netz, *PNAS* 105, 2842 (2008)

[3] Polypeptide friction and adhesion on hydrophobic and hydrophilic surfaces: A molecular dynamics case study, A. Serr, D. Horinek and R.R. Netz, *Journal of the American Chemical Society* 130, 12408 (2008)