IMPRS on Multiscale Biosystems

Title: A molecular-scale workbench for bio-nanoparticles
PI: Prof. Svetlana Santer (UP) or Prof. Peter Saalfrank (UP)*
In collaboration with: Prof. Peter Saalfrank (UP) or Prof. Svetlana Santer*, Dr. Mark Santer (MPIKG)

Project description: Manipulating single nano-scale objects such as proteins, strands of DNA or colloids is a fascinating and promising, but also difficult endeavor. Although with the various techniques of atomic force microscopy one can have detailed looks at nano objects, placing and possibly relocating them is a nuisance. This project is about establishing a "pin board" for bio-nanoparticles that may be used to temporarily attach objects at defined locations, and possibly detach them later on. To achieve this, functionalized substrates will be employed with molecularly thin films of photosensitive groups that can be tuned with respect to their adhesive properties by illumination with external light. An example are azobenzene monolayers on Si-substrates (see figure), undergoing trans-cis isomerization and changes of their dipole moment upon illumination.

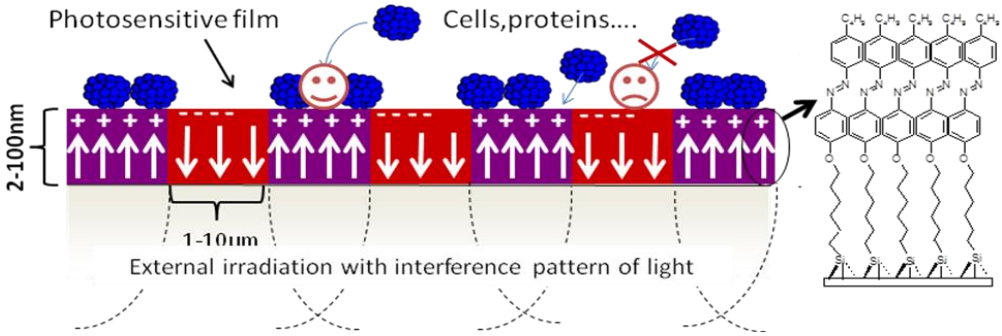

Figure 1. Scheme of the biomolecular pin board (left), realized by an array of photo-switchable molecules (right).

The student will fabricate functionalized substrates using modern prototyping techniques, and investigate the adsorption of cells, proteins etc. with atomic force microscopy and other methods. The interpretation of experimental results also requires insights on atomistic length scales. Which kind of substrate allows for very fast switching? Why does one kind of photosensitive molecule works better than another? The student will learn and use methods from quantum chemistry (density functional theory, non-adiabatic dynamics "on the fly"), as well as molecular dynamics that not only complement experimental data but also could lead to suggestions for new molecular "designs".

*Depending on the student's background and interests, either the experimental work (PI Santer) or the theoretical aspects (PI Saalfrank) can be the focus of the thesis

Required background: The prospective student should have a background in physical and/or theoretical chemistry or physics.

Paper to read before the interview:

1. Santer, S et al., "DNA compaction by azobenzene-containing surfactant" *Phys Rev E*, 84 (**2011**) 021909
2. Füchsel, G. et al. "On the electronic structure of neutral and ionic azobenzenes and their possible role as surface-mounted molecular switches", J Phys. Chem. B, 110 (2006) pp. 16337

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