

Upgrading the devices we use every day requires solving deep scientific problems. The proposed project is an example showing that despite the long-term motivation lying in applied science area, the real goal is aimed at understanding the basic rules of a physical phenomenon.

The application motivating our research lies in many applications of titania (TiO_2), such as photocatalysis and development of dye-sensitized solar cells (DSSC) proposed by O'Regan and Grätzel in 1991. DSSCs, for instance have been intensively studied since then since they have some important advantages over the semiconductor-based cells. In DSSCs light is adsorbed in large organic molecules adsorbed on the surface of an electrode. The connection between a molecule and an electrode must allow for effective charge transfer. And often is one of the bottlenecks limiting the efficiency of a device.

During the development of DSSC technology materials most suitable for electrodes were selected. The most common is the surface made of nanoparticles of TiO_2 in the form of rutile and anatase. Dyes used are usually aromatic molecules with quite a large spectrum of light adsorption. The molecules are equipped with moieties which should allow for efficient charge transfer from a molecule to an electrode, as well as for stable anchoring of a molecule. As the result, the efficiency of a device depends strongly on the morphology of molecules deposited on the substrate.

To predict and improve the quality of molecular layers we have to understand the rules guiding the adsorption and organization of molecules. In the case of rutile there is quite a lot of microscopic data available describing how the relevant molecules are forming the adlayers. As for anatase, there is hardly any. That is because it is quite difficult to prepare atomically clean surface of single crystal anatase. Since we have learnt how to do it, we may start to explore the adsorption behavior of selected molecules.

We have selected three porphyrines with different number of anchoring, carboxylic groups and three different phthalocyanines with different metal atoms in the molecular structure. This will allow us to check the two main factors in forming molecular adlayers: the role of the most commonly used anchoring group and how the type of metal affects the molecular organization. Since we are interesting in tiny amount of molecules (no more than two monolayers) the study will be performed by the use of scanning probe microscopy (SPM), accompanied by x-ray photoelectron spectroscopy for gaining the additional insight into the molecule-substrate interaction.