Hybrid Inorganic/Organic Systems for Opto-Electronics

Collaborative Research Centre 951

HIOS

Colloquium Announcement

of the Collaborative Research Centre 951 “Hybrid Inorganic/Organic Systems for Opto-Electronics”

Egbert Zojer

Institute of Solid State Physics, Graz University of Technology, NAWI Graz, Austria

The impact of polar layers on the electronic properties of organic/inorganic hybrid interfaces

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Stefan Kirstein

Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin

HIOS based on nanotubular J-aggregates

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Collaborative Research Centre 951
Department of Physics
Humboldt-University of Berlin

Email: sfb951@physik.hu-berlin.de
Tel.: +49 30 2093 66374
www.physik.hu-berlin.de/sfb951

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The impact of polar layers on the electronic properties of organic/inorganic hybrid interfaces

Egbert Zojer

Institute of Solid State Physics, Graz University of Technology, NAWI Graz,
Petersgasse 16, 8010 Graz, Austria

The presence of polar layers crucially determines the electronic properties of essentially all technologically relevant interfaces. In my presentation, I will start with discussing their fundamental properties paying particular attention to the differences between isolated dipoles and collective electrostatic effects caused by periodic dipole assemblies. The latter directly impact important interface quantities, like the sample work function and the relative alignment of the electronic states in the substrate and the adsorbate.

The possible origins of those dipole layers are manifold, where generally one has to distinguish between dipoles already present in the adsorbed molecules and dipoles that arise from interfacial charge rearrangements or distortions of the adsorbed molecules during interface formation. Of particular interest beyond the omnipresent Pauli-Pushback caused by exchange interactions are system-specific charge rearrangements triggered by the adsorption of particularly electron-rich (donors) or electron-poor molecules (acceptors). For these, depending on the degree of electronic coupling between the substrate and the adsorbate, one has to distinguish between fractional charge transfer, where each of the adsorbed molecule donates or accepts a fractional number of electrons, and integer charge transfer, where a fraction of the adsorbed molecules receive an integer charge. In both situations, the interface enters the realm of Fermi-level pinning, in which the sample work function becomes essentially independent of the substrate (i.e., the work function of the used metal) and is solely determined by the electronic properties (in particular the ionization energy and the electron affinity) of the adsorbate layer. Notably, the latter typically differ fundamentally from the respective properties of the isolated molecules, as they are strongly influenced by the orientation of dipole moments situated in the molecular periphery. Therefore, changes in the adsorbate structure can trigger massive work-function shifts at metal/organic interfaces, even if the molecules per se do not possess any dipole moments.

On more practical grounds, dipole-induced work-function shifts can be used for tuning charge-carrier injection barriers, where I will discuss, how the adsorption of polar moieties can be used to change contact resistances of electrodes by several orders of magnitude making Au a suitable contact metal not only for hole- but also for electron-injection into organic thin-film transistors. Besides work functions and injection barriers, the presence of polar layers can modify a multitude of additional physical observables, which will be discussed for core-level binding energies and tunneling currents through monolayer junctions.

Finally, if time permits, I will also briefly explain, how the inevitable consequences of dipolar layers on the electronic structure of interfaces can be used to create materials with unprecedented properties in the spirit of an “electrostatic design of materials”.

HIOS based on nanotubular J-aggregates

Katherine Herman, Egon Steeg, Holm Kirmse, Jürgen P. Rabe, Stefan Kirstein

Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

The main objective of our project (A6) is to develop quasi one-dimensional HIOS based on highly ordered nanotubular J-aggregates of amphiphilic cyanine dyes, which readily self-assemble in solution. The HIOS shall be obtained either by chemical in situ synthesis or by physical adsorption of pre-fabricated inorganic semiconductor nanocrystals. It is one of our goals to fabricate a HIOS that allows to investigate the exciton migration length within these aggregates. One approach is to add two separate Förster-transfer couples to the aggregates where the mutual distance between acceptor and donor can be varied. This was intended by adding semiconducting nanocrystals to the aggregates that serve as donors and acceptors [1]. For successful fabrication it became necessary to first produce aggregates homogeneously covered by a polyelectrolyte that serves as a glue. Previous work has shown that the surface of the tubes can be coated with oppositely charged polyelectrolytes without altering the optical properties of the aggregate [1]. The optimization of this procedure will be described and discussed. Another approach is to investigate single, isolated aggregates on a substrate to use microscopic techniques to study the exciton migration. We now try to extend the idea of electrostatic based assembly to form silica coatings capable of stabilizing the aggregates for investigations in environmental or even low pressure conditions. The recent progress with this respect will be presented.

Additionally, the growth of wires within the aggregates was studies further. These wires grow after addition of silver nitrate to the solution and were initially described as silver nanowires [2,3]. Since these wires were thought to be used for plasmon applications, their properties were studied furthermore in detail. It was found by structure analysis of single wires that they actually consist of silver iodine, a finding that was completely surprising [4]. These data will be presented and discussed as well.

References:

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[2] Eisele, D.M.; von Berlepsch, H.; Böttcher, C.; Stevenson, K.J.; Vanden Bout, D.A.; Kirstein, S.; and Rabe, J.P., J. Am. Chem. Soc. **132**, 2104 (2010)

[3] Steeg, E.; Polzer, F.; Kirmse, H.; Qiao, Y.; Rabe, J.P.; Kirstein, S., Journal of Colloid And Interface Science **472**, 187-194 (2016)

[4] Steeg, E., Kirmse, H., Rabe, J.P., Kirstein, S., Journal of Colloid and Interface Science **530**, 424-432 (2018)