Hybrid Inorganic/Organic Systems for Opto-Electronics

Sonderforschungsbereich 951

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des Sonderforschungsbereichs 951 „Hybrid Inorganic/Organic Systems for Optoelectronics"

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Theory and Simulation of Electronic Structure and Energy Conversion at Inorganic-Organic Interfaces

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The Growth of Inorganic Nanowires in Tubular J-Aggregates

Zeit: Donnerstag, den 28.06.12, 16:00 Uhr s.t.
Ort: Erwin-Schrödinger-Zentrum, Rudower Chaussee 26, Raum 0'119.

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Theory and Simulation of Electronic Structure and Energy Conversion at Inorganic-Organic Interfaces

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New materials, architectures, and concepts are needed to realize many low-cost, sustainable energy conversion applications. Nanostructures are highly promising in this respect. Distinguished by their large surface-to-volume ratios, nanostructures frequently lead to, upon integration into assemblies and devices, a high density of active hybrid interfaces that are central to function. In this talk, I will describe the development and application of predictive theoretical and computational approaches, based on density functional theory and beyond, to the study of physical structure and electronic energy level alignment at inorganic-organic interfaces of relevance to energy conversion phenomena. Specific interfaces to be discussed include single-molecule junctions, donor-acceptor systems in organic solar cells, and organic ligands on semiconductor nanostructures and photocatalysts.

The growth of inorganic nanowires in tubular J-aggregates

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The use of organic supra-molecular assemblies as soft templates for the growth of inorganic materials is a well established method to form nano-structured objects. The wide variety of supramolecular structures provides the possibility to tailor the size and shape of inorganic nanomaterials by low-sophisticated techniques.

Here, tubular J-aggregates that are built by amphiphilic carbocyanine dyes in aqueous solutions are used as templates for the growth of wire-like inorganic structures. The J-aggregates self-assemble into very regular tubes with a typical diameter of 13 nm and length exceeding micrometers [1]. These aggregates are of interest not only because of their structure but also due to their outstanding optical properties that are caused by the strong excitonic coupling. Here, we show further functionalization of these aggregates, either by attachment of different dye groups at the outside of the aggregates, or by growth of inorganic systems inside the tubes. As an example, growth of silver nanowires within the tubes is obtained by reduction of silver salt [2]. Thereby, the wires fill the inner volume of the tubular aggregates with a diameter of 6.5 nm and grow in length up to several hundred nanometers. The growth of the wires is observed at different time steps using electron microscopy in order to conclude on the nucleation process. This principle of template synthesis was applied to other materials such as ZnO, ZnS, and CdS. Preliminary results will be presented that clearly show the success of this method, as long as the chemical reactions take place at room temperature. The prospective but also the draw backs of this method will be discussed.

[1] Eisele, D. M.; Knoester, J.; Kirstein, S.; Rabe, J. P.; Vanden Bout, D. A., Nature Nanotechnology, 4, 658 (2009);

[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)