



Colloquium Announcement

of the Collaborative Research Centre 951

“Hybrid Inorganic/Organic Systems for Opto-Electronics”

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**Two-dimensional π -conjugated networks:
Electronic properties and impact of lattice
symmetry**

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**Active control of electro/optical interface properties
in hybrid inorganic/organic systems**

Time: Thursday, April 26, 2018, 3 pm c.t.

Place: Erwin-Schrödinger-Zentrum, Rudower Chaussee 26,
Room 0`119.



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Two-dimensional π -conjugated networks: Electronic properties and impact of lattice symmetry

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In this presentation, we will first give a brief introduction to the field of two-dimensional π -conjugated covalent organic frameworks (COFs).

In the context of the collaborations we have with our experimental partners (Will Dichtel at Northwestern; Seth Marder and Phillip First at Georgia Tech; Mike Crommie and Feng Wang at Berkeley; and Dan Ralph at Cornell), we will describe the results of the electronic-structure calculations as well as molecular-dynamics and kinetic Monte Carlo simulations we have carried out on monolayers of two-dimensional π -conjugated polymer networks based on three-arm and four-arm cores. We will detail how the symmetry of the core units and of the lattice influences the nature of the electronic bands at/near the Fermi energy, which can go from being totally flat to being highly dispersive. We will discuss the implications this has namely with regard to charge transport. Finally, we will describe the interfaces formed between such two-dimensional conjugated-polymer monolayers and substrates such as gold or boron nitride.

This work is conducted in the framework of the ARO-MURI Center for Advanced 2D Organic Networks (CATON).

Active control of electro/optical interface properties in hybrid inorganic/organic systems (HIOS)

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This contribution will give an overview of current results and activities of the B14 project of CRC 951. The goal of this project as a whole is to expand the concept of hybrid inorganic/organic systems (HIOS) introducing optically switchable molecules such as dihydropyrene (DHP) and diarylethenes (DAE) on inorganic semiconductors or metal structures.

In the first part of this contribution, we report on the switching process of the photochromic molecules DAE and DHP on different surfaces (ZnO and ITO). Probing the electronic density of states (DOS) and changes at the electronic energy landscape by means of photoemission and optical spectroscopy, we investigate the molecular films both in form of self-assembled monolayers (SAMs) as well as in bulk thin films. We find that the isomeric switch leads to an optically induced energy level shift of the highest occupied molecular orbitals (HOMO) of DAE as well as DHP molecules with respect to the Fermi level (E_F). These modifications of the HOMO level may then be used to control the energy level alignment in diode structures.

In the second part of this contribution we report on the optically switchable DHP molecules with varying dipole moment. We discuss the resonant coupling between plasmonic excitations of metallic substrates and DHP using differential transmission and reflectance spectroscopy aimed at modulating the propagation of coupled plasmonic excitations at the HIOS interface.