

HL 46: Organic Semiconductors

Time: Wednesday 9:30–11:30

Location: H13

HL 46.1 Wed 9:30 H13

Exciton-Polaritons in Open Organic Microcavities — ●SIMON BETZOLD, CHRISTOF P. DIETRICH, and SVEN HÖFLING — Technische Physik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg

Frenkel excitons, characteristic of organic semiconductors, possess large binding energies and are stable at room temperature, making polariton experiments at ambient air conditions feasible. Organic materials further exhibit very large oscillator strengths and thus strongly interact with a cavity field. Circumventing the issue that organic materials are very sensitive to the depositing of semiconductor layers on top of them, we use an open cavity system, which makes non-invasive investigation of the active material possible.

Open cavities are tunable systems and comprise a bottom semiconductor distributed Bragg reflector (DBR) with the active material (the organic semiconductor) on top and a concave top DBR separated by a micrometer sized air gap. This configuration allows a 3D photonic confinement and brings unprecedentedly high quality factors into reach.

Here, we show the versatility of open cavities by performing reflectivity and photoluminescence measurements in Fourier imaging configuration and exemplarily investigate the strong exciton-photon coupling between a red-emitting polymer and the dielectric cavity. We emphasize that the open cavity approach can easily be extended to more complex active regions including two-dimensional monolayer materials or hybrid organic-inorganic bilayers.

HL 46.2 Wed 9:45 H13

Multi-scale modeling of spin transport in organic semiconductors — ●AMAURY SOUZA¹, SHAYAN HEMMATIYAN¹, ERIK MCNELLIS¹, DENIS ANDRIENKO², and JAIRO SINOVA¹ — ¹Johannez Gutenberg University - Mainz — ²Max Planck Institute for Polymers - Mainz

In this work, we present our theoretical framework to simulate simultaneously spin and charge transport in amorphous organic semiconductors. By combining several techniques e.g. molecular dynamics, density functional theory and kinetic Monte Carlo, we are able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in a realistic morphology of amorphous organic systems. We apply our multi-scale approach to investigate the spin transport in amorphous Alq₃ (Tris(8-hydroxyquinolino)aluminum) and address the underlying spin relaxation mechanism in this system as a function of temperature, bias voltage, magnetic field and sample thickness.

HL 46.3 Wed 10:00 H13

Conformal growth of ultra-thin p-conductive polymer layers on n-type semiconductor nanostructures by oxidative chemical vapour deposition — ●LINUS KRIEG¹, STEPHANIE BLEY², MAX RÜCKMANN², JÜRGEN GUTOWSKI², FLORIAN MEIERHOFER³, LUTZ MÄDLER³, and TOBIAS VOSS¹ — ¹Institute of Semiconductor Technology and LENA, Braunschweig University of Technology — ²Institute of Solid State Physics, Semiconductor Optics, University of Bremen — ³Foundation Institute of Material Science, Department of Production Engineering, University of Bremen

Inorganic-organic hybrid systems consisting of conjugated polymers and inorganic semiconductors are promising for the development of cheap, versatile and tailored electronic and optoelectronic devices. A gentle approach for polymer layer deposition is offered by the oxidative chemical vapour deposition (oCVD), a solventless and dry method where the oxidising agent and the monomer are provided in the gaseous phase. In our experiments, we use FeCl₃ as an oxidising agent and monomers of the p-conductive polymers polypyrrole (PPy) and poly(3,4-ethylenedioxythiophene) (PEDOT) to conformally coat n-type ZnO and GaN wafers and nanowires. SEM and TEM measurements confirm that we can achieve conformal coating of the entire nanowire with the conductive polymer while the optical properties of the inorganic semiconductors show no substantial deterioration. The layer thickness is in the order of a few tens of nanometres and can be controlled by the total amount of the oxidising agent provided during the coating process.

30 min. Coffee Break

HL 46.4 Wed 10:45 H13

α,ω -Dihexyl-sexithiophene thin films for solution-gated organic field-effect transistors — ●HANNAH SCHAMONI¹, SIMON NOEVER², BERT NICKEL², MAX KRAUT¹, MARTIN STUTZMANN¹, and JOSE A. GARRIDO³ — ¹Walter Schottky Institut und Physik-Department, Technische Universität München, Deutschland — ²Fakultät für Physik und CeNS, Ludwig-Maximilians-Universität München, Deutschland — ³Catalan Institute of Nanoscience and Nanotechnology, CSIC and The Barcelona Institute of Science and Technology, Barcelona, Spain

While organic semiconductors are being widely investigated for chemical and biochemical sensing applications, major drawbacks such as the poor device stability and low charge carrier mobility in aqueous electrolytes have not yet been solved to complete satisfaction. In this work, solution-gated organic field-effect transistors (SGOFETs) based on the molecule α,ω -dihexyl-sexithiophene are presented as a promising platform for in-electrolyte sensing. It is shown that the performance of the SGOFETs can be improved by choosing suitable growth parameters which lead to a two-dimensional film morphology and a high degree of structural order. Furthermore, the capability of the SGOFETs to detect changes in the pH or ionic strength of the gate electrolyte is demonstrated and successfully simulated. Excellent transistor stability is confirmed by continuously operating the device over a period of several days. Altogether, our results demonstrate the feasibility of high performance and highly stable organic semiconductor devices for chemical or biochemical applications.

HL 46.5 Wed 11:00 H13

Correlation of Crystalline Structure and Optical Properties of Perylene: a Comprehensive Experiment-Theory Comparison — ●ANDRE RINN¹, TONATIUH RANGEL², ANDRÉ PICK¹, GREGOR WITTE¹, LEEOR KRONIK³, JEFFREY NEATON², and SANGAM CHATTERJEE¹ — ¹Faculty of Physics, Philipps Universität Marburg, Renthof 5, D-35032 Marburg, Germany — ²Molecular Foundry, Lawrence Berkeley National Laboratory, University of California, Berkeley, 1 Cyclotron Road, MS 67R3207 Berkeley, CA 94720, U.S.A. — ³Faculty of Chemistry, Weizmann Institute of Science, Rehovot 76100, Israel

Aromatic molecules such as perylene and its derivatives find wide spread usage in electronic devices and as dyes as this class of material shows strong light-matter coupling. Here, we show a comprehensive study of the optical properties of the model semiconductor perylene. It adopts two distinctive crystalline polymorphisms, both of which show vastly different excitonic structure and carrier dynamics. The comparison of a detailed theoretical analysis based on first-principles calculations with the polarization-resolved experimental linear absorption spectra yields excellent agreement. In particular, we discuss the importance of electron-hole interaction effects beyond a standard two-particle picture and implications of different approximations commonly made in calculations using density functional theory and many-body perturbation theory formalisms.

HL 46.6 Wed 11:15 H13

Strain and Pressure Dependent Electronic Properties of Polyacetylene — ●FRANZ KNUTH¹, CHRISTIAN CARBOGNO¹, VOLKER BLUM², and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — ²MEMS Department, Duke University, Durham, NC 27708, USA

Strain, stress, and pressure can influence the electronic properties of organic semiconductors [1]. In this contribution, we present the changes of electronic and transport properties for crystalline *trans*-polyacetylene under strain and hydrostatic pressure in the framework of density-functional theory. We critically discuss the role of approximations in the exchange-correlation functional and show that the fraction of exact exchange included in the calculations with hybrid functionals is non-trivial to choose and essential for the correct description of polyacetylene. The pressure studies are performed with the help of the analytical strain derivatives (stress tensor) including the contributions coming from van-der-Waals corrections and exact exchange [2]. Our calculations also reveal that the electronic band structure and gap of polyacetylene are not only determined by the dimerization of the carbon chain but are at least as much influenced by interchain

interactions.

[1] J. H. Kim, S. Seo, and H. H. Lee, Appl. Phys. Lett. **90**, 143521

(2007); G. Giri *et al.*, Nature. **480**, 504 (2011)

[2] F. Knuth *et al.*, Comp. Phys. Comm. **190**, 33 (2015)