

CPP 36: Organic Electronics and Photovoltaics IV

Time: Thursday 15:00–16:00

Location: H38

CPP 36.1 Thu 15:00 H38

How to Capture and Release Fullerene from an Azobenzene-Bithiophene Nanolayer? — DMITRY A. RYNDYK and ●OLGA GUSKOVA — IPF Dresden, Hohe Str. 6 01069 Dresden

Optimizing organic photovoltaic devices involves the strategic use of well-defined monolayers of azobenzene-bithiophene (Azo-BT) switches. These monolayers serve as a bridge between inorganic and organic components, allowing precise nanoscale control over electrode morphology [1]. Previous studies have demonstrated that cis- and trans-Azo-BT switches chemisorbed on a gold surface exhibit distinct geometrical, electronic, and charge transport properties. We further investigate the behavior of cis- and trans-Azo-BT monolayers, with a particular focus on "nanotraps" nanometer-sized nanopores formed within the monolayers and their ability to capture&release fullerene. Our findings confirm that the photoswitchable "closed" and "open" configurations of Azo-BT nanotraps remain stable at room temperature under experimentally relevant surface densities. Energy calculations reveal that C60 molecules preferentially stabilize inside the open nanotrap near the pore surface, effectively capturing the fullerene. Additionally, a local energy minimum for C60 near the electron-donating BT block suggests charge transfer from the BT fragment to the fullerene, enhancing the interaction between the trap and the captured molecule. To expel the fullerene from the monolayer, we applied an alternating voltage electric field and determined the optimal parameters required to displace the nanoparticle, demonstrating the feasibility of controlled capture and release. [1] Savchenko, V. et al., *Processes*, 11 (2023) 2625.

CPP 36.2 Thu 15:15 H38

Deciphering vibronic interactions in NDI-T2 based donor-acceptor type oligomers with theoretical and experimental spectroscopy — ●MAXIMILIAN F.X. DÖRFNER¹, MARKO MEDUGORAC¹, AJEET KUMAR², JÜRGEN HAUER¹, and FRANK ORTMANN¹ — ¹TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany — ²Department of Chemistry, Lund University, Naturvetarvägen 14 222 62 Lund, Sweden

In this study, we investigate the alternating Naphthalendiimide-bithiophene co-oligomer (T2-NDI2OD-T2), a fundamental building block of the high charge-mobility polymer-semiconductor PNDI(2OD)2T. This class of materials has garnered significant attention for its exceptional charge transport properties, making it a promising candidate for applications in field-effect transistors and as non-fullerene acceptors in organic photovoltaics. We use Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT) to examine the ground and singlet excited state properties to understand the electronic structure and vibrational excitations. Additionally, we analyze the coupling between electronic and vibrational degrees of freedom by means of a Linear Exciton-Vibrational Coupling Model parameterized by DFT. We compare the computed optical observables to the experiment and discuss the role of molecular vibrations in this system.

CPP 36.3 Thu 15:30 H38

Grain Boundaries and Charge Mobility in Organic Semiconductors: A Non-Adiabatic Molecular Dynamics Approach — ●SONALI GARG¹, FARHAD GHALAMI¹, SEBASTIAN SCHELLHAMMER², and MARCUS ELSTNER¹ — ¹Karlsruhe Institute of Technology, Karlsruhe, Germany — ²Technische Universität Dresden, Germany

Organic semiconductors have emerged as crucial materials in the development of electronic and optoelectronic devices due to their exceptional mechanical flexibility, lightweight nature, and cost-effectiveness. However, the presence of grain boundaries (GBs) can significantly impede device performance by introducing traps or potential barriers that reduce charge carrier mobility. This study investigates the influence of the GB characteristics, including misorientation angles and GB width, on charge carrier mobility and compares the results with intrinsic mobility. Non-Adiabatic Molecular Dynamics (NAMD) simulations, employing Fewest Switches Surface Hopping (FSSH) approach[1,2,3], were used to model charge transport dynamics. The charge transfer Hamiltonian was constructed using a fragment orbital approach, with its elements computed via the Density Functional Tight Binding (DFTB) method[4,5]. These insights provide a deeper understanding of the effects of GB on charge carrier mobility in organic semiconductors.

[1]Spencer. J et al. *J. Chem. Phys.* (2016) [2]Roosta. S *J. Chem. Theory Comput.* (2022) [3]Xie. W et al. *J. Chem Theory Comput.* (2020) [4]Elstner. M et al. *Phys. Rev. B* (1998) [5]Kubař. T et al. *J. Phys. Chem. B* (2010)

CPP 36.4 Thu 15:45 H38

Single-particle spectra of pentacene from exact simulations of Green's functions in the time-domain — ●MICHEL PANHANS¹, FRANK ORTMANN¹, and HIROYUKI YOSHIDA² — ¹TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany — ²Graduate School of Engineering, Chiba University, 1-33 Yayoicho, Inage-ku, Chiba, 263-0043, Japan

The investigation of single-particle spectra using experimental techniques such as photo-electron spectroscopy and inverse-photoelectron spectroscopy reveal the nature of the charge carriers close to the Fermi energy. In particular for organic crystals such as pentacene, the single-particle spectra are strongly affected by the electron-phonon coupling (EPC) and crucially deviate from the theoretical spectra based on ab initio band-structure calculations associated with the HOMO and the LUMO of the pristine crystal.

To model these experiments more accurately, Green's-function approaches including the EPC are a suitable methodology to describe what is seen in experiments. In our present study, we calculated the HOMO and the LUMO spectra of pentacene single-crystals and compared them to experimental results. We find that the quantum mechanical treatment of the EPC has a crucial impact on the fine structure of the spectra and explains the band features of the experimental spectra for HOMO and LUMO of pentacene.