Invited Talk HL 86.1 Thu 15:00 H34

Quantum coherence controls the charge separation in a proto-type artificial light harvesting core complex. C. Falke1, S. M. Falke2, C. A. Rozzi3, N. Spallanzani4, A. Rubó4, E. Molinari5, D. Brida6, M. Mairini7, G. Cerullo8, H. Schramm9, and J. Christoffers10 — 1Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — 2Institut Nanosciences - CNR, Centro S3, Modena, Italy — 3IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy — 4Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The efficiency conversion of light into electricity or chemical fuels is a fundamental challenge. In artificial photosynthetic and photovoltaic devices this conversion is generally thought to happen on ultrafast time scales, in the fs to ps range and to involve an incoherent electron transfer process. In some natural biological systems, however, there is now growing evidence that the coherent motion of electronic wavepackets is an essential primary step, raising questions about the role of quantum coherence in artificial devices. Here we investigate the primary charge transfer process in a supramolecular triad, a prototypical artificial reaction center. Combining high time-resolution femtosecond spectroscopy and time-dependent density functional theory, we provide compelling evidence that the driving mechanism of the photoinduced current generation cycle is a correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. We highlight the fundamental role of the interface between chromophore and charge acceptor in triggering the coherent electron-hole wave splitting.

Simulations of Electron Transfer in a Fullerene Hexa-Pyropheophorbide-a Complex — Thomas Pfehn, Jörg Mégow, and Volkhard May — Humboldt-Universität zu Berlin, Germany

Electron transfer (ET) is studied between electronically excited chromophores and a C60 fullerene forming a highly flexible complex, which is dissolved in a solvent. Such investigations are of particular interest with regard to future artificial photosynthetic reaction centers and respective applications in future components of photovoltaic devices. The whole discussion is based on extended MD-simulations. To obtain reliable ET results three differently advanced theories are used. The first treatment uses the classical Marcus theory. Respective Marcus parameters are obtained from literature [1]. A generalized ansatz can be derived by the Landau-Zener theory [2]. Secondly, a semi-classical surface-hopping method [3] is chosen. For this approach the conformation-dependent free-energy surfaces and Marcus parameters are calculated directly from the MD-trajectory. The third approach uses the dispersed-polaron/spin-boson model [3]. This method enables the characterization of a quantum-mechanical harmonic oscillator bath and thus the treatment of nuclear tunneling. A comparative discussion of the outcome of these three methods also in relation to experiment [1] is given finally.


Highly conductive PEDOT:PSS for flexible structured ITO-free solar cells — Claudia M. Palumbiny1, Christoph Heller1, Robert Meier1, Gonzalo Santoro2, Stephen V. Roth3, and Peter Müller-Buschbaum4 — 1Institut Nanosciences - CNR, Centro S3, Modena, Italy — 2IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy — 4Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

PEDOT:PSS is widely used as selective intermediate electrode in flexible electronics. The mechanical stability of the electrodes yet play a crucial role and is limited by the instability of the ITO/FTO electrode and the low conductivity of PEDOT:PSS. We investigate a recently developed post treatment method enhancing the conductivity of PEDOT:PSS reaching the order of ITO. For a deeper understanding the nanomorphology is investigated with surface imaging techniques (AFM, SEM) and the inner morphology and crystallinity is addressed with GISAXS and GIWAXS. The morphological changes are consequently related to the electronically changes. Furthermore, we introduce a novel structuring routine for PEDOT:PSS, plasticizer assisted soft embossing [1]. Being able to control the interface between the transparent electrode and the active material is a key requirement of OPVs under oblique light can be increased. Combining highly conductive PEDOT:PSS with controlled structuring, these results reveal new paths for flexible structured ITO-free solar cells of enhanced efficiency.

Enhanced light outcoupling from corrugated top-emitting OLEDs — C. Fuchs, T. Schwan, A. Zakhyndov, K. Leo, M. C. Gather, and R. Scholz.

We analyse the emission spectra of phosphorescent top-emitting OLEDs grown on corrugated substrates. The corrugation is produced using photolithography. Thereby photoresist, spin-coated on a glass substrate is illuminated by an incoherent UV source across a contact mask with periodic structures in the sub-μm range. The optical micro-cavity of the OLED grown on top is defined by a thick metallic bottom contact, organic layers following the p-i-n concept, a thin metallic top contact, and an organic capping layer maximizing the outcoupling efficiency. Depending on the periodicity of the substrate, Bragg scattered wave guide modes may interfere constructively or destructively with the cavity mode inside the air light cone, hence enhancing or decreasing light emission with respect to a planar microcavity. Thus, the emission pattern deviates strongly from a Lambertian shape, but the angle-integrated external quantum efficiency can be enhanced by up to a factor of about 1.2 with respect to a fully optimized planar reference. Besides a quantitative assignment of sharp features in the emission spectra, an analysis of Bragg scattering for different periodicities can be used for designing a particular angular emission pattern, e.g. very strong forward characteristics.


In this work we present the fabrication, characterization and ink formulation of gravure printed polymer light-emitting electrochemical cells (LEC). These light emitting devices are fabricated by sandwiching a blend of a semiconducting polymer with a solid polymer electrolyte (SPE) between two electrodes, regardless of their work function. When applying a voltage to the device, the ionic species in the active film will help to form p or n doped layers at the corresponding electrode. Following the injection of carriers, the light emission will come from the semiconductor through the formation and successive recombination of excitons in the intrinsic layer between the p and n doped regions. We compare the LEC ink formulation to the film quality and device performance. The properties of the formulation are characterized by viscoscosity and contact angle measurements while the properties of the film are studied by impedance spectroscopy and atomic force microscopy.
One-dimensional wires constituted with kinds of segments attracted much attention due to their potential application in nanogaps obtained from on-wire lithography, plasmonic disk arrays, optimized Raman *hot spots* and heterojunction structures1. Here, we will talk about the in-wire device, which combined the organic semiconductor and the electrodes in an individual nanowire, based on anodic alumina oxide (AAO) template2-3. This kind of nanodevice could be applied in organic diodes, transistors or memories, which attracted extensive attention due to the flexibility, the ease to be functionalized, the colorful and the low cost4.

Reference: