



APRIL 27-29, 2015 GERMAN-THAI WORKSHOP ON PHOTOVOLTAICS

OPV – OLED – DSSC

This spring, researchers from German and Thai institutions will meet in Mülheim to discuss their recent results and to establish further collaborations on experiments and simulations of organic-photovoltaic materials and devices. **Lectures Open to the Public**



Max-Planck-Institut für Kohlenforschung
The Light and Molecules Group



Speakers

W Arbelo-González
I Dokukina
N Elfers
D Fazzi
S Jungsuttiwong
N Kungwan
S Namuangruk
V Promarak
JD Spiegel
T Sudyoadsuk
T Very

Organizers

M Barbatti
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Program & Information
barbatti.org/gtw2015

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German-Thai Workshop on Photovoltaics

Venue

- Max-Planck-Institut für Kohlenforschung
Kaiser-Wilhelm-Platz 1
45470 Mülheim Ruhr Germany

Date

- April 27-29, 2015

Organizers

- MARIO BARBATTI
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Steady and Time-Resolved Ionization Spectrum Simulations

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The calculation of photoionization spectra in polyatomic molecules has been included as a new functionality into the Newton-X package [1]. Working as an extension of the nuclear ensemble approach [2], the method provides spectra with vibrational broadening beyond the Condon approximation, and will serve as basis for simulations of time-resolved photoelectron spectra. The approach we have implemented involves (1) the selection of an ensemble of nuclear configurations, according to a given scheme that parallels the experimental conditions as close as possible, (2) the computation of the Dyson orbitals, i.e., the single electron wave functions defined as the overlap between electronic states of the N and $N-1$ electron species and (3) the calculation of the ionization cross-sections [3] for each nuclear geometry generated. In this work, we formally present the methodological aspects regarding each of these points, in particular within the frame of linear response time-dependent density functional theory. As an illustrative example of the capabilities of our method, the comparison between the photoionization spectrum of dimethyl sulfide, $S(CH_3)_2$, calculated by us and measured in recent experiments is discussed.

[1] M. Barbatti, M. Ruckebauer, F. Plasser, J. Pittner, G. Granucci, M. Persico, and H. Lischka, *WIREs: Comp. Mol. Sci.*, **4**, 26 (2014).

[2] R Crespo-Otero, and M. Barbatti, *Theor. Chem. Acc.*, **131**, 1237 (2012).

[3] C. Melania Oana, and A. I. Krylov, *J. Chem. Phys.*, **131**, 124114 (2009).

QM/MM at a Test: The Isomerization of Retinal in Channelrhodopsin

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Channelrhodopsins (ChRs) are light-gated cation channels derived from algae that have shown experimental utility in optogenetics. [1] Upon light absorption, photoisomerization of their cofactor retinal triggers activation of the channel. ChRs can be genetically introduced into cells to modulate and examine neuron activity in living tissues non-invasively. [2] Despite successful applications in optogenetics, they still have limitations for certain biological applications. [3] Enhancement of their functionality requires detailed knowledge of photo- and thermally induced reactions. Yet, little is known about structural and spectral characteristics of intermediates within the ChR photocycle.

To study this subject we apply a combined quantum mechanical/molecular mechanical (QM/MM) approach implemented in COBRAMM. [4] This scheme allows investigation of ground and excited state properties of dyes in various environments employing a subtractive QM/MM protocol. The molecule of interest is described at a quantum chemical level, while the environment is treated with less demanding molecular mechanics methods. Special care needs to be taken at the connection points of the two areas; we use a link atom scheme which saturates dangling QM bonds with a hydrogen atom. The molecular wave function is polarized by MM atomic point charges (electrostatic embedding). [5]

For our investigation we used the crystal structure of C1C2 channelrhodopsin, a chimera of channelrhodopsin-I and channelrhodopsin-II from *Chlamydomonas reinhardtii*. Ground state geometries were obtained for different models of dark-adapted ChR with all-*trans* retinal and the first photointermediate with a 13-*cis* retinal configuration. Vertical excitation energies were calculated using multiconfigurational single state/multi state-CASPT2 and DFT/MRCI methods. Experimental values for the first excited state in dark-adapted ChR have been reproduced with good accuracy, calculations for the first intermediate will give insight into the mechanism of the following proton transfer reaction. Since retinal photoisomerization is a central event in channel activity, we want to explore reaction routes inducing this process. Currently our work is focused on calculation of the all-*trans* \rightarrow 13-*cis* (Fig. 1) Minimum Energy Path (MEP), considering different amino acid protonation states. MEPs are computed at CASSCF and CASPT2 levels. Spectroscopic properties of optimized structures are compared to experimental data.

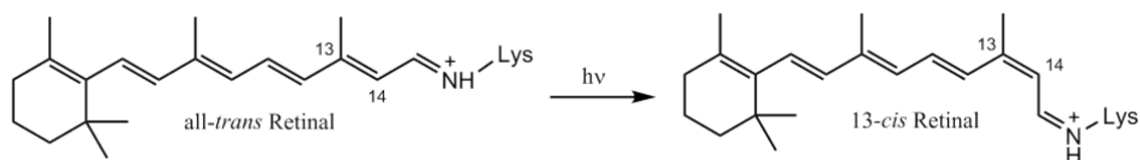


Figure 1: all-*trans* to 13-*cis* retinal photoisomerization

[1] Kato, HE., Nureki, O. et al., *Nature* 482 (2012) 369 - 374.

[2] Kamiya, M., Hayashi, S. et al., *Chem. Phys. Lett* 556 (2013) 266 - 271.

[3] Hegemann, P., Möglich, A., *Nat. Methods* 8 (2011) 39 - 42.

[4] Altoè, P., Stenta, M., Bottoni, A., Garavelli, M. *Theor. Chem. Acc.* 118 (2007) 219 - 240.

[5] Polli, D., Rivalta I., Nenov, A., Weingart, O., Garavelli M. and Cerullo, G. *Photochem. Photobiol. Sci.* 2015, in print, DOI: 10.1039/c4pp00370e

Singlet Fission in Quinoidal Bithiophene

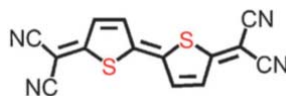
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Quinoidal oligothiophenes are of great interest in the development of organic semiconducting materials. Because of their diradical character and low-lying triplet states they are also interesting candidates for singlet fission, a process in which a singlet exciton is divided into two triplet excitons. Thus, the efficiency of organic solar cells could be increased to overcome the Shockley Queisser Limit [1].

In this work, the ground state and excited singlet and triplet states of quinoidal tetracyano bithiophene (TCQBT) are calculated in order to investigate its ability to undergo singlet fission.

As a simple model for a molecular crystal we looked at a dimer of two pi-stacking molecules of TCQBT. Their geometry has been optimized using density functional theory including dispersion interactions (DFT-D3) [2]. Potential energy curves corresponding to the pi-stacking distance for the ground state and low-lying singlet and triplet states are presented. For calculating the excited states, multi-reference perturbation theory (MRMP2) [3] is employed. Here we use Kohn-Sham-Orbitals for the calculations because they describe the virtual space much better than Hartree-Fock-Orbitals at relatively low computational cost compared to e.g. CASSCF. Orbitals obtained by the BHLYP-functional have shown to yield the best results.



The adiabatic electronic states are analyzed to show that TCQBT meets the energetic requirement for the process of singlet fission: $E(S_1) \geq 2E(T_1)$. Furthermore, we can identify a dark singlet state with high double excitation character, which can be interpreted as a coupled triplet pair.

Vibronic couplings between the bright singlet state and the dark doubly excited state are calculated.

¹ J. Casado, R. P. Ortiz, and T. López Navarrete, *Chem. Sov. Rev.* **2012**, 41, 5672-56876.

² S. Grimme, J. Antony, S. Ehrlich, and H. Krieg *J. Chem. Phys.* **2010**, 132, 154104

³ S. Grimme and M. Waletzke, *Phys. Chem. Chem. Phys.* **2000**, 2, 2075-2081.

Ultrafast Processing and Molecular Understanding of Organic Solar Cells

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The understanding of the electronic structure at the donor/acceptor (D/A) interface and the primary mechanisms of exciton deactivation in organic materials, plays a key role in organic photovoltaics. These aspects determine the evolution of the photoinduced species, having a direct impact on the power conversion efficiency of the solar cell [1]. For this reason, accurate predictions of D/A electronic structure [2], and the ultrafast relaxation mechanisms [3], has become nowadays as much valued as urgent.

In this work, we investigate both aspects, adopting state-of-the-art Density Functional Theory (DFT) calculations and nonadiabatic excited states dynamics methods [4].

Excited states at the D/A interface of the most efficient (co)polymers/PCBM blends (Figure 1a) are computed and classified on the basis of their localization, delocalization and charge transfer (CT) character.

We found that the size of the D/A supramolecular cluster, and the relative position of the PCBM with respect to the polymer co-units, affect the interplay between CT vs. localized states, and their spatial extension.

Exciton-relaxation dynamics are investigated in a series of oligothiophenes, representing the best model for P3HT. Photorelaxation takes place through a cascade of ultrafast nonadiabatic transfers amongst the manifold of excited states, and for the longest oligothiophene considered, we predict an exciton localization mechanisms occurring within 150 fs (Figure 1b), in perfect agreement with the experimental data for P3HT. In the frame of photovoltaics, this implies that any exciton-dissociation process has to happen on a time scale faster than 200 fs [3].

Our investigations give insight in the molecular understanding of photovoltaic processes, with the aim to boost the efficiency of organic solar cells starting from a rational chemical-physical design.

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[2] K. Sen, R. Crespo-Otero, O. Weingart, W. Thiel, M. Barbatti, *J. Chem. Theory Comput.*, **2013**, *9*, 533–542.

[3] G. Grancini, M. Maiuri, D. Fazzi, A. Petrozza, H. J. Egelhaaf, D. Brida, G. Cerullo and G. Lanzani, *Nature Materials*, **2013**, *12*, 29-33.

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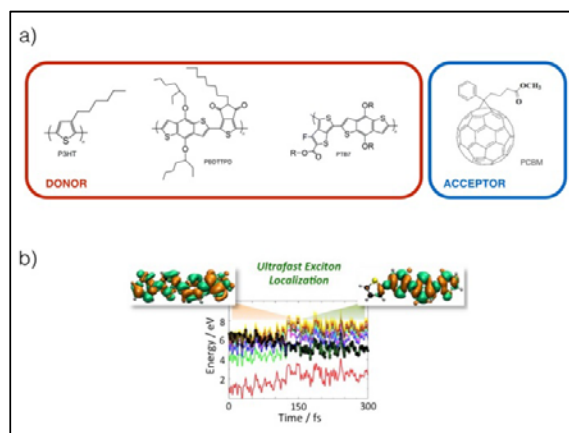


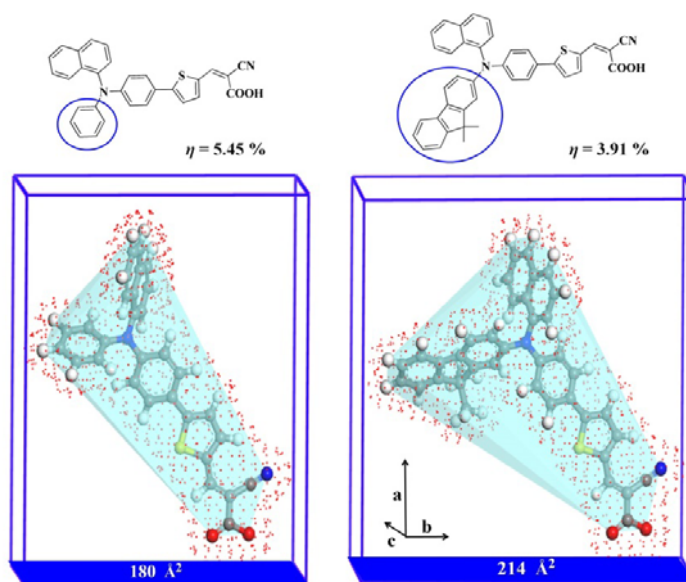
Figure 1: a) chemical structure of donor and acceptor compounds; b) ultrafast exciton localization for tetrathiophene

The Number Density Effect of N-Substituted Dyes on the TiO₂ Surface in Dye Sensitized Solar Cells: A Theoretical Study

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A series of organic dyes, containing N-Substituted carbazole, diarylamine-naphthalene, and diarylamine-fluorene donor is successfully investigated by DFT and TDDFT. Among these dyes, **Dye3**, with the strongest electron donating ability, shows the most red shift in the UV-Vis absorption spectrum. Moreover, **Dye3**@(TiO₂)₃₈ complex shows stronger adsorption energy of -19.54 kcal/mol. Nevertheless, **Dye2** has shown the best photovoltaic performance. We measured the molecular volume and molecular width to investigate the effect of N-substituted donors on the number density of the adsorbed dye, on the TiO₂ surface. We found that the bulkiness of the N-substituted donor in **Dye3** can dramatically reduce the number density of the adsorbed on the surface. The molecular width and projected area of **Dye3** are calculated to be 15.980 Å of 214 Å², respectively, indicating the more bulky-structure compared to **Dye2** which corresponds to the dye uptake of **Dye3** (1.38×10^{17} molecule cm⁻²) is significantly less than **Dye2** (4.55×10^{17} molecule cm⁻²). Finally, **Dye3** with extra-bulky donor exhibits poorer energy conversion efficiency of 3.91% compared to 5.45% of **Dye2**, under simulated AM 1.5 irradiation (100 mW cm⁻²).



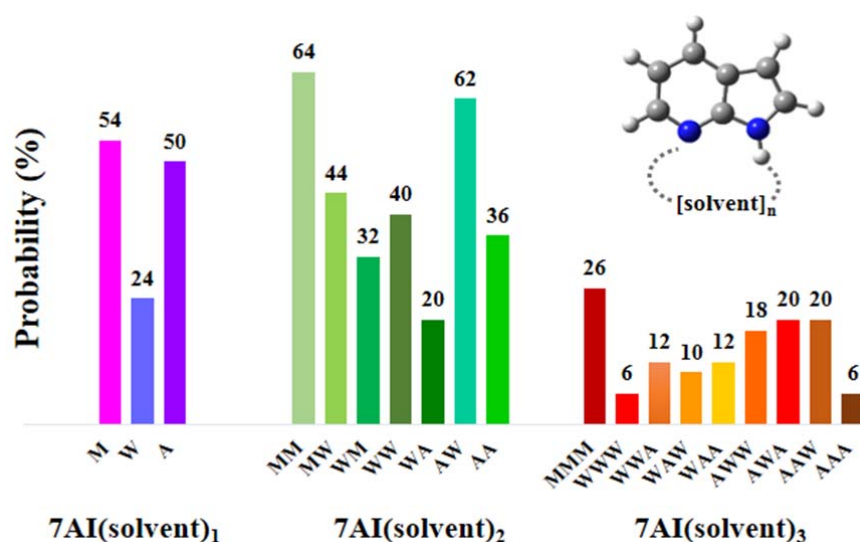
Keywords: Density functional theory (DFT), N-substituted donors, Molecular volume, Molecular width

Excited-State Proton Transfer Reactions of 7-Azaindole with Water, Ammonia and Mixed Water-Ammonia: Microsolvated Dynamics Simulation

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Dynamics simulations of excited-state multiple proton transfer (ESMPT) reactions in 7-azaindole (7AI) with ammonia, mixed water-ammonia, and water molecules were investigated by quantum dynamics simulations in the first-excited state using RI-ADC(2)/SVP-SV(P) in the gas phase. 7AI(WW), 7AI(WA), 7AI(AW), and 7AI(AA) clusters (W-Water and A-Ammonia) show the very high probability of the excited-state triple proton transfer (ESTPT) occurrence in ranges from 20% for 7AI(WA) to 60% for 7AI(AW), respectively. Furthermore, 7AI(AW) clusters with ammonia placed near N-H of 7AI has the highest probability among other isomers. In 7AI with bridge-planar solvent of water, ammonia, and mixed water-ammonia clusters, the excited-state quadruple proton transfer (ESQPT) reactions rarely occur. In particular, replacing H₂O with NH₃ assists ESMPT corresponding to lower barrier in the excited state. Base assistance plays crucial role in the ESTPT in presence of low barrier in the excited state.



DFT Study of the Fructose to 5-Hydroxyl-Methylfurfural on the External H-ZSM-5 (001) Surface

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Zeolites have been reported as effective catalysts for conversion of fructose to 5-hydroxymethylfurfural (5-HMF), which is an important chemical building block in biomass conversion processes. In this work, we carried out the density functional theory (DFT) calculations to investigate the reaction mechanism of β -D-fructose conversion to 5-HMF over the H-ZSM-5 zeolite (001) surface modelled by the 34T cluster representing Si/Al ratio of 34. The mechanism was proposed as four elementary steps in sequence: 1) the first dehydration of β -D-fructose, 2) the enol-keto tautomerization process, 3) the second dehydration, and finally 4) the third dehydration to form the 5-HMF product. The obtained results suggested that the third step is the rate-determining step with the activation energy of 54 kcal/mol. This result is in good agreement with the experimental observation ($E_{app} = 50$ kcal/mol) using the H-ZSM-5 zeolite with high Si/Al ratio. The DFT results suggest that the 2nd dehydration (the removal of water from the aldehyde-intermediate) is the most difficult in process.

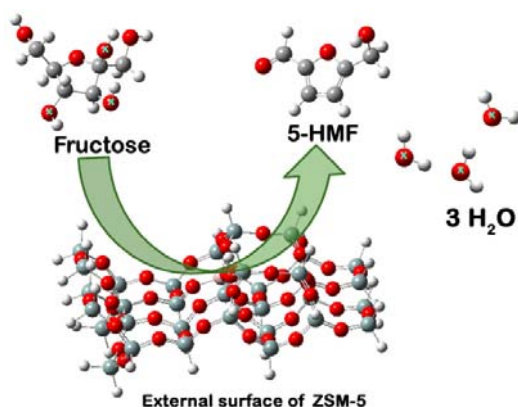


Figure. Dehydration of three water molecules from fructose to 5-HMF over external surface of H-ZSM-5 (001).

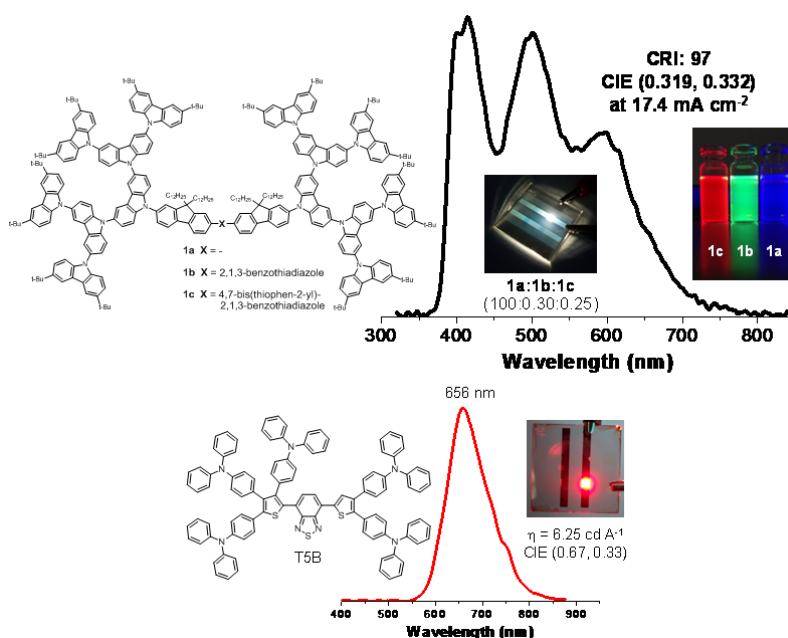
Keywords: Fructose, 5-HMF, Dehydration, H-ZSM-5, DFT

The Designs of Solution-Processed Hole-Transporting Non-Doped Emitters for Efficient Organic Light-Emitting Diodes (OLEDs)

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A series of triphenylamine-functionalized bis(thiophenyl)benzothiadiazoles and carbazole dendrimers containing different types of fluorescent cores were synthesized and characterized as non-doped solution-processed hole-transporting light-emitters for OLED. They displayed a bright fluorescence and could form morphologically stable amorphous thin films with high glass transition temperatures. Simple structured solution-processed OLEDs using these materials as hole-transporting non-doped emitters emitted stable emission with high luminance efficiencies (up to 9.12 cd A^{-1}). The CIE coordinates of emitted colors of red, green and blue OLEDs were (0.63, 0.36), (0.27, 0.62) and (0.17, 0.11), respectively, which are close to the pure RGB colors. These compounds as bifunctional material also showed great ability as hole-transporting material for Alq3-based green OLED with a high luminance efficiency (5.63 cd A^{-1}). Solution-processed WOLED based on these RGB dendrimers exhibited a high luminance efficiency (3.06 cd A^{-1}) with a high color rendering index (CRI) of 97. The performance of such OLEDs is comparable with or better than existing OLEDs with the advantage of the simple fabrication method.



Keywords: carbazole dendrimer, bis(thiophenyl)benzothiadiazoles, non-doped emitter, solution processed, organic light-emitting diode

Molecular Design of Donor- π -Acceptor Type Organic Dyes for Efficient Dye-Sensitized Solar Cells

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Dye-sensitized solar cells (DSSCs) have been intensively investigated since the report of highly efficient ruthenium complex-sensitized TiO₂ solar cells by the Swiss scientists. To date, overall conversion efficiencies of up to 12% were achieved from the ruthenium complex device. However, pure organic dyes exhibit not only higher extinction coefficient, but simple preparation and purification procedure with a low cost. Recently, enormous progress has been made in this field and the highest overall photoelectric conversion efficiency of solar cells sensitized by organic dyes containing an electron donor (D) and an electron acceptor (A), separated by a π -conjugation bridge (π) has reached 13%. This indicates the promising perspective of metal-free organic dyes [1].

In my talk, a series of novel D- π -A type organic dyes bearing carbazole or porphyrin as electron donor moiety (D), oligothiophene segments with number of thiophene units from one to three units as π -conjugated spacers (π) and cyanoacrylic acid as the electron acceptor (A) have been synthesized and characterized as dye sensitizers for DSSCs [2-6]. These compounds exhibit high thermal and electrochemical stability. Detail investigations of these dyes reveal that both peripheral donor moieties not only can contribute electron injection into TiO₂ upon photo-excitation, either directly or indirectly by internal conversion to the lowest excited state, but also inhibit aggregation between dye molecules and prevent iodide/triiodide in the electrolyte from recombining with injected electrons in the TiO₂, leading to increased overall conversion efficiency. The overall efficiencies of the corresponding devices reach 98% with respect to that of the N3-based device fabricated and measured under similar conditions. This work suggests that the organic dyes based on this type of donor moiety or donor molecular architecture are promising candidates for improvement of the performance of the DSSCs.

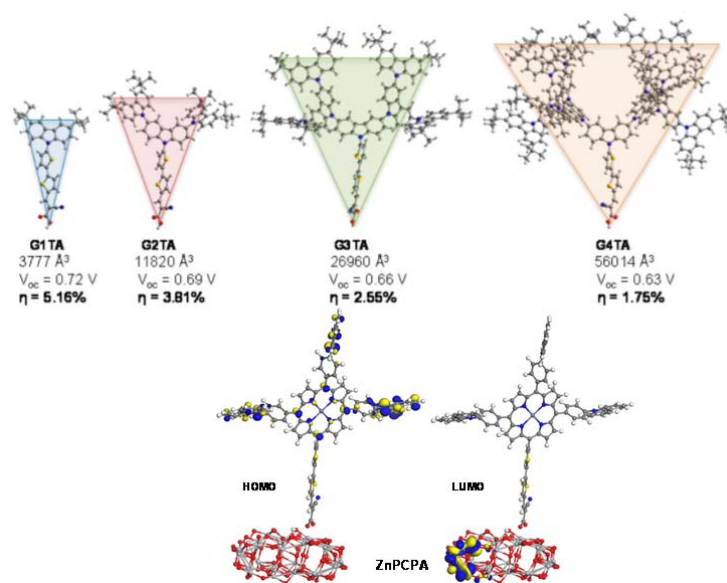


Fig 1. D- π -A type dyes and the DFT calculation.

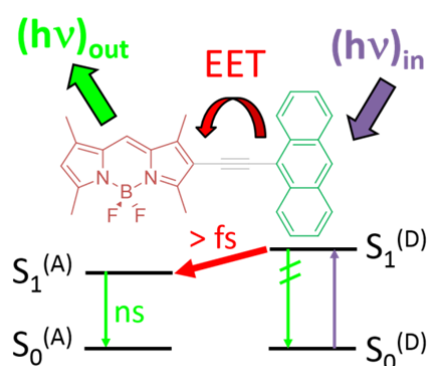
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Energy Transfer Processes in BODIPY-based Donor-Acceptor-Systems

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In organic solar cells, the photoexcitation energy is transferred in a very fast process from the reception layer to its interface area with the electron transport layer where charge separation takes place. The exciton transport can be described as excitation energy transfer (EET) between adjacent monomeric units. 4,4-Difluoro-4-bora-3a,4a-diaza-s-indacene- (BODIPY) based energy transfer systems are promising acceptors in bulk heterojunction solar cells¹.



In this work we examined the through-space contribution of EET in a set of BODIPY-based energy transfer cassettes with quantum chemical methods. Excitonic couplings were calculated using both Ideal Dipole Approximation (IDA)² and Monomer Transition Density Approach (MTD).³ EET rates were calculated according to Fermi's Golden Rule from excitonic coupling and spectral overlap of the emission spectrum of the donor and the absorption spectrum of the acceptor.

For intermolecular distances larger than 10 Å excitonic coupling can be described with both IDA and MTD with equal accuracy. At closer distances the IDA fails while the MTD approach still provides reasonable results. The error of the IDA is particularly large when the donor acceptor distance is small and the transition dipole moments are situated in a parallel manner. We found that the exchange contribution of the excitonic coupling is negligible in all studied energy transfer systems. The calculated EET rates are higher $5.0 \times 10^{-12} \text{ s}^{-1}$ and confirm the experimental findings of Kim *et al.*⁴

¹ A. M. Poe *et al.*, *Chem. Comm.* 50 (2014), 2913-2915.

² C. Y. Wong *et al.*, *J. Chem. Phys.* 130 (2009), 081104.

³ R. F. Fink *et al.*, *Chem. Phys.* 346 (2008) 275-285.

⁴ T.G. Kim *et al.*, *J. Phys. Chem. A* 110 (2006) 20-27.

Simulation of Organic Bulk Heterojunction Current-Voltage Curve

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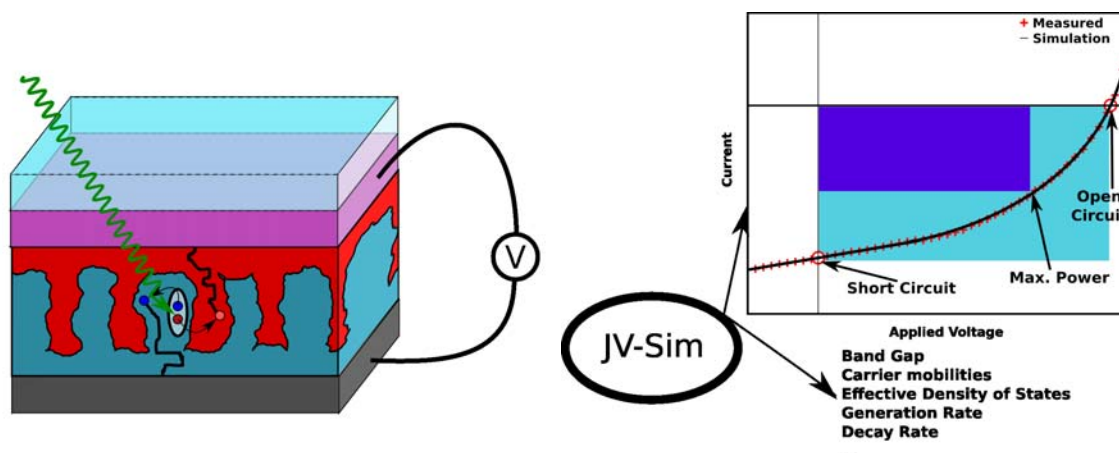
One of the major challenge of our and future generations is to find new ways of energy production to replace fossil/nuclear fuel.

A promising technology is based on organic polymers and molecules that conduct electricity upon light irradiation. Especially we are interested in Bulk Heterojunction (BHJ) [1] devices where an electron acceptor (usually a fullerene derivative) and an electron donor (usually a conducting polymer) are mixed and sandwiched between two electrodes.

Researchers are looking at different pathways ranging from the study of electronic properties of organic systems at the molecular level to the behavior of complete devices. Here we focus on the mesoscopic scale by studying the active layer of one cell.

One way to measure the efficiency of solar cells is to plot the current density against the applied voltage on the cell. From this plot we apply a device model [2] that relies on several parameters that we can determine by using a fitting procedure.

Finally, we can use the parameters to complete the necessary rational design of novel conducting molecules.



[1] Heeger, A. J. (2014). 25th anniversary article: Bulk heterojunction solar cells: understanding the mechanism of operation. *Advanced Materials* (Deerfield Beach, Fla.), 26(1), 10–27.

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Notes

Notes

Program

| | Mon 27.04 | Tue 28.04 | Wed 29.04 |
|---------------|-----------------|---------------|-----------|
| 10:00 – 11:00 | PROMARAK | | M1 |
| 11:00 – 11:40 | ELFERS | KUNGWAN | M2 |
| 11:40 – 12:20 | ARBELO-GONZÁLEZ | NAMUANGRUK | M3 |
| 12:20 – 14:00 | Lunch | | |
| 14:00 – 14:40 | VERY | DOKUKINA | M4 |
| 14:40 – 15:20 | FAZZI | JUNGSUTTIWONG | M5 |
| 16:00 – 16:40 | SPIEGEL | SUDYOADSUK | M6 |

M – Group meetings and lab visits

Public lectures: 40 min (25-30 min talk + discussions)

Topics and Speakers

Calculation of Photoionization Spectra with Newton-X:

Details on the Implementation and Application

WILMER ARBELO-GONZÁLEZ – *Max-Planck-Institut für Kohlenforschung*

QM/MM at a Test: The Isomerization of Retinal in Channelrhodopsin

IRINA DOKUKINA – *Heinrich Heine Universität Düsseldorf*

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Ultrafast Processing and Molecular Understanding of Organic Solar Cells

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The Number Density Effect of N-Substituted Dyes on the TiO₂ Surface in Dye Sensitized Solar Cells: A Theoretical Study

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Energy Transfer Processes in BODIPY-Based Donor-Acceptor Systems

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Simulation of Organic Bulk Heterojunction Current-Voltage Curve

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