



**Hybrid Inorganic/Organic Systems
for Opto-Electronics**

Sonderforschungsbereich 951



HIOS Young Researcher Workshop 2020

**18-19 November 2020
Online Workshop**

Book of Abstracts



Collaborative Research Centre 951
Department of Physics
Humboldt-Universität zu Berlin

Email: sfb951@physik.hu-berlin.de
Tel.: +49 30 2093 66380
www.physik.hu-berlin.de/sfb951

Partners



Schedule

Wednesday (18.11.20)	Thursday (19.11.20)
<p style="text-align: center;">Opening Remarks 10:00 – 10:15</p>	<p style="text-align: center;">Exciton Dynamics 10:00 – 11:00</p> <p style="text-align: center;">Jannis Krumland (B16) Olga Turkina (B11) Dominik Christiansen (B12) Hélène Seiler (B17)</p>
<p style="text-align: center;">CRC 951 Overview 10:15 – 10:45</p> <p style="text-align: center;">Emil List-Kratochvil (B14)</p>	<p style="text-align: center;">Coffee Break 11:00 – 11:30</p>
<p style="text-align: center;">Coffee Break 10:45 – 11:15</p>	<p style="text-align: center;">Plasmonics 11:30 – 12:00</p> <p style="text-align: center;">Günter Kewes (B18) Dan-Nha Huynh (B10)</p>
<p style="text-align: center;">Organic Semiconductors: Optical & Electronic Properties 11:15 – 12:00</p> <p style="text-align: center;">Alexander Neef (B17) Dominique Lungwitz (A8) Boubacar Tanda Bonkano (B9)</p>	<p style="text-align: center;">Family and career support during the COVID-19 pandemic 12:00 – 12:20</p> <p style="text-align: center;">Maurizio Roczen (Z3)</p>
<p style="text-align: center;">Lunch Break 12:00 – 13:00</p>	<p style="text-align: center;">Lunch Break 12:20 – 13:20</p>
<p style="text-align: center;">Poster Session 13:00 – 14:30</p>	<p style="text-align: center;">TMDCs: Optical & Electronic Properties 13:20 – 13:50</p> <p style="text-align: center;">Patrick Amsalem (A8) Sven Lubeck (B11)</p>
<p style="text-align: center;">Coffee Break 14:30 – 15:00</p>	<p style="text-align: center;">Perovskites 13:50 – 14:20</p> <p style="text-align: center;">Cecilia Vona (B11) Giovanni Procida (B16)</p>
<p style="text-align: center;">Fundamental Investigation Methods 15:00 – 16:00</p> <p style="text-align: center;">Johannes Müller (A12) Kyrylo Greben (B15) Samuel Palato (B9) Alaa Akkoush (A13)</p>	

Sessions

Wednesday:

- 10:00 am **Opening Remarks**
- 10:15 am **CRC 951 Overview: Emil List-Kratochvil**
Chair: Seon-Young Rhim
- 11:15 am **Organic Semiconductors: Optical & Electronic Properties**
Chair: Thorsten Schultz
- 01:00 pm **Poster Session**
- 03:00 pm **Fundamental Investigation Methods**
Chair: Patrick Amsalem

Thursday:

- 10:00 am **Exciton Dynamics**
Chair: Matheus Jacobs
- 11:30 am **Plasmonics**
Chair: Dominik Christiansen
- 12:00 pm **Family and career support during the COVID-19 pandemic**
Chair: Alaa Akkoush
- 01:20 pm **TMDCs: Optical & Electronic Properties**
Chair: Alaa Akkoush
- 01:50 pm **Perovskites**
Chair: Florian Mathies

Poster Session

18.11.2020 (Wed.), 01:00-02:30 pm

Nr.	Presenter	Title
1	Alberto Eljarrat	Studying SPR mode dispersion and temporal coherence in dye-embedded silica-covered Ag-NWs
2	Dmitrii Maksimov	Ab initio structure search of (flexible) molecules at interfaces
3	Dragos Mutruc	Modulating Guest Uptake in Core-Shell MOFs with Visible Light
4	Hu Lin	Reversible Switching of Charge Transfer at the Graphene-Mica Interface with Intercalating Molecules
5	Ignazio Gonzales	Electron-phonon coupling in hybrid inorganic/organic systems: implementation within the LAPW formalism
6	Kristin Klaue	Donor-Acceptor Dihydropyrenes Switchable with Near Infrared Light
7	Manuel Katzer	Charge and Energy Transfer in Bilayer TMDCs and Hybrid Molecule-TMDC Structures
8	Marcel Schloz	Overcoming information reduced data and experimentally uncertain parameters in ptychography with regularized optimization
9	Martin Rothe/ Yuhang Zhao	Local-chirality sensors for HIOS from self-assembled plasmonic nano-antenna-waveguide structures
10	Matheus Jacobs	Ultrafast charge transfer and vibronic coupling in donor/acceptor interfaces from first principles
11	Meysam Raoufi	Probing the charge carrier dynamics in hybrid layer stacks comprising a TMDC monolayer and an organic semiconductor
12	Nicolas Zorn Morales	Switching impact of photochromic diarylethenes as self-assembled monolayers in organic light emitting diodes
13	Pauline Liesfeld	Highly Cooperative Photoswitching in Dihydropyrene Dimers
14	Raymond Amador	Electronic and optical properties of Na ₂ KSb and NaK ₂ Sb from ab initio many-body theory
15	Richard Schier	Electronic and optical properties of BCF-doped oligothiophenes from ab initio many-body theory
16	Rika Simon	Structural and electronic properties of F6-TCNQ on monolayers of MoS ₂ investigated by STM/AFM
17	Ronaldo Pela	All-electron real-time TDDFT implementation with Ehrenfest molecular dynamics
18	Seon-Young Rhim	Waveguide mode modulation with photochromic molecules for neuromorphic computing
19	Stefano Calati	Dynamic Screening of Quasiparticles in WS ₂ Monolayers
20	Victoria Taylor	Ultrafast spectroscopy and ultrafast electron diffraction studies of perovskites

Important Information at a glance

ZOOM links:

The workshop will be held via ZOOM with the talks and poster sessions being held in separate ZOOM rooms. Please click on the links below for direct access to the corresponding ZOOM room or use the provided log-in data. The login data will not change during the workshop.

Program	ZOOM link	Meeting ID	Password
Oral presentations	Link	661 5070 2456	065908
Poster sessions	Link	690 0966 0758	065908

Please make sure to download the latest version of ZOOM. More technical information on ZOOM can be found on the next page.

Communication with other participants:

During the oral presentations, the chat function will be limited to communication with the hosts (speaker, chair, moderators) of the session.

During the breaks the chat will be open to all participants. If you wish to have a private break out room with other participants, please send Seon-Young Rhim or Yuhang Zhao a private message via the chat function.

During the poster sessions, you will be able to chat with all participants of the conference.

ZOOM basics:

Audio/Video: By clicking on the buttons "Join Audio" and "Start Video" in the lower left corner of the ZOOM window you can activate and deactivate your video/audio, respectively. Please keep both deactivated during the oral presentations unless you receive a notification to do otherwise.

Screen Sharing: To share your screen, click on the green button "Share Screen" in the lower middle of the ZOOM window.

The "raise hand" feature: To raise your hand, click on the "Participants" button in the lower middle of the ZOOM window. The participants window will open. In the bottom of this window, you have several buttons for nonverbal feedback, including the "raise hand" button.

The Chat function: To chat with other participants, click on the "Chat" button next to the "Share Screen" button in the lower middle of the ZOOM window. The chat window will open. In the lower area of the chat window is the input field. Right above the input field, you can choose if you want to address your message to all participants or only to certain participants (during the oral presentations, you can only write to the hosts of the meeting).

Technical advice for using ZOOM:

Please make sure to use the latest ZOOM version. If possible, use a LAN connection instead of WiFi, especially if you plan to activate your camera or audio. This notably improves your video and audio quality. If possible, try to minimize background noise when activating your audio and avoid rooms with a large echo. Your audio quality can be further enhanced by using a headset.

Oral Presentations

The first oral presentation on Wednesday, 18th November 2020, starts at 10:00 am.

The first oral presentation on Thursday, 19th November 2020, starts at 10:00 am.

General Information

After entering the ZOOM room, your microphone and camera will be deactivated. We kindly ask you to keep both deactivated at all times, unless the moderators ask you to activate them. The speakers will share their screens for their presentations. For the best possible view, we recommend to hide participants without video and to activate the side-by-side-mode.

Discussions

Your questions and comments are highly welcome after the talk. For this, you have the following two options:

- **Use the "raise hand" feature:** you can ask your question in person after the talk by using the "raise hand" feature. You will receive a notification to activate your microphone and camera (if applicable) which you have to do manually. After your question was answered, please deactivate your microphone and camera again and lower your hand.
- **Ask your question in the chat:** you can write down your question at any time in the chat and send it to the session chair who will read your question aloud after the talk. Please refrain from writing to the speaker directly. If possible, start writing your question during the talk.



Personal Information:

Name: Alexander Neef

Project: B17

Office number: (030)-8413 5149

e-mail: neef@fhi-berlin.mpg.de

Momentum-resolved singlet fission

Alexander Neef, Samuel Beaulieu, Shuo Dong, Tommaso Pincelli, Julian Maklar, Patrick R. Xian, Laurenz Rettig, Martin Wolf and Ralph Ernstorfer

Abstract:

Converting solar energy in silicon is limited to an efficiency of $\approx 30\%$ by the Shockley-Queisser limit [1]. This limit can be increased to $\approx 45\%$ by exploiting singlet fission (SF) [2], a mechanism in which an excited singlet state \mathbf{S}_1 is converted to two triplet states $2\mathbf{T}_1$. In this work, we investigate SF in rubrene crystals using time- and angle-resolved photoemission spectroscopy (trARPES) [3] and show the momentum-resolved dynamics of \mathbf{S}_1 and \mathbf{T}_1 . This allows us to extract information about the spatial extent of the two states.

References:

- [1] W. Shockley, H. Queisser, *J. Appl. Phys.* **32**, 510 (1961).
- [2] M. B. Smith, J. Michl, *Chem. Rev.* **110**, 6810 (2010).
- [3] M. Puppin *et al.*, *Optics Express* **23**, 1491 (2015).

**Personal Information:****Name:** Dominique Lungwitz**Project:** A8**Office number:** (030) 2093-7534**e-mail:** lungwitz@physik.hu-berlin.de

Single step production of a self-organized, low work function cathode interlayer from polymer blend solution

Dominique Lungwitz, Keli Fabiana Seidel, Andreas Opitz, Thomas Krüger,
Jan Behrends, Seth R. Marder and Norbert Koch

Abstract:

The application of cathode interlayer in order to reduce the work function of electrodes is a widely studied method in organic electronic devices. Here, we report a simple procedure to obtain a self-organized interlayer on indium-tin oxide (ITO) electrode from a blend solution of poly[N,N'-bis(2-octyldodecyl)naphthalene-1,4,5,8-bis(dicarboximide)-2,6-diyl]-alt-5,5'-(2,2'-bithiophene) [P(NDI2OD-T₂)] and polyethylenimine (PEI). A self-organized interlayer is formed from blend solution due to vertical phase separation of the polymers during film drying. The measured energy level alignment reveals the presence of n-type Fermi level pinning of P(NDI2OD-T₂) at PEI covered ITO electrodes and thereby the lowest possible electron injection barrier. Furthermore, an increased charge carrier density was measured. Finally, we conclude that the reduction of interfacial electron trapping and changes in morphology are the main reasons for the observed increase in polymer conductivity. The results show clearly that films processed from sequential deposition or blend solution must be in-depth studied to differentiate between work function reduction upon interfacial layers and conductivity increase upon changes of structural conformation [1].

References:

- [1] K. Seidel, D. Lungwitz, A. Opitz, *et al.*, ACS Appl. Mater. Interfaces **12**, 28801-28807 (2020).



Personal Information:

Name: Boubacar Tanda Bonkano

Project: B9

Office number: (030) 8413-5130

e-mail: tandabonkano@fhi-berlin.mpg.de

Excited state dynamics of unsubstituted terrylene, a textbook molecule

Boubacar Tanda Bonkano, Björn Kobin, Sergey Kovalenko, Stefan Hecht and Julia Stähler

Abstract:

In hybrid solar cells, the separation of the electron-hole pairs after photogeneration is a key aspect of the light-harvesting process. This requires, in hybrid inorganic/organic systems, the use of molecules that have excited states with sufficiently long lifetime to allow charge separation. In order to investigate terrylene molecules, we performed two types of time-resolved spectroscopy, time-correlated single photon counting (TCSPC) and broadband transient absorption (TA) using a white light continuum probe. The steady state absorption and emission of terrylene molecules in solution show mirrored lineshapes displaying a clear vibronic progression. Both the TCSPC and TA consistently show a decay of 3.7 ns for the excited state S_1 . Terrylene thin film shows a significant change of the absorption properties likely due to H-aggregation.¹⁻² The measurement of the thin films shows, in addition to the known ns dynamics, spectral components with dynamics three orders of magnitude faster than in the single molecule.³ Studying the physical mechanisms arising from these aggregates is challenging but yet necessary for a better understanding and the control of terrylene related systems, beneficial for applications.

References:

- [1] Arundhati P. D., Danielle Koppel, *et al.*, J.Phys. Chem. C **133**, 18702 (2019).
- [2] Nicholas J. Hestand, and Frank C. Spano, Chem. Rev. **118**, 7069 (2018).
- [3] Eric A. Margulies, *et al.*, J. A. CHEM. Soc. **139**, 663 (2016).



Personal Information:

Name: Johannes Müller

Project: A12

Office number: (030) 2093-7734

e-mail: johannes.mueller@physik.hu-berlin.de

Enabling imaging and spectroscopy of electron beam sensitive hybrid materials

Johannes Müller, Benedikt Haas, Alberto Eljarrat and Christoph T. Koch

Abstract:

We modified our scanning electron microscope (SEM) to acquire diffraction patterns of thin samples in transmission. By analyzing the acquired diffraction patterns, we can investigate crystallographic and material properties on mm^2 -scale with a spatial resolution of less than 5nm [1], for example how organic and inorganic components of HIOS are orientated with respect to each other. The SEM offers low acceleration voltages (0.5-30kV) reducing knock-on beam damage to the sample and increasing elastic scattering yielding stronger contrast compared to higher electron energies. We can map with up to 2000 diffraction patterns per second while scanning the electron beam over the sample, giving the A12 project a fast and easy to use system to investigate HIOS.

Our future plans are to use a direct camera, resulting in single electron sensitivity reducing sample damage and possible contaminations. We are also planning to implement electric field mapping and diffraction in reflection, which will allow us to investigate samples on top of substrates without the otherwise necessary sample preparation.

With the installation of our new Nion electron microscope, we can now investigate atomic and electronic structure, interface charges, phonons, defects and many other material properties using the sub-angstrom spatial resolution and the $<5\text{meV}$ energy resolution.

References:

- [1] B. Haas, J. Müller, J. L. Rouvière and C. T. Koch, *Imag. & Micros.* **3/2019**, 35 (2019).



Personal Information:

Name: Kyrylo Greben

Project: B15

Office number: (030) 838-61110

e-mail: k.greben@fu-berlin.de

In situ functionalization of two-dimensional materials

Kyrylo Greben, Sebastian Thalheim, Sviatoslav Kovalchuk and Kirill Bolotin

Abstract:

An attractive strategy to create new types of 2D matter is to functionalize defect sites in original 2D materials. However, freshly-generated defects react in the ambient environment. This greatly reduces the applicability of defect-engineering approaches to functionalization of 2D materials.

Here we explore the controlled chemical functionalization of defects inside 2D materials in a vacuum environment and at cryogenic temperatures. We constructed the set-up that combines *in-situ*: 1) local high-temperature annealing of 2D materials kept at cryogenic vacuum, 2) generation of functional and structural defects by means of controllable RF-plasma, 3) doping and surface functionalization using gasses and organic molecules, and 4) measurement of the Raman and photoluminescence (PL) spectra of various 2D materials.

In graphene, we generated more than 10^{13} cm^{-2} defects and found that they are functional and very reactive. We then performed the two-step proof-of-principle *in-situ* functionalization of freshly-generated functional defects using the ammonia functional [1].

In TMDCs, we used *in-situ* deposition of oxygen molecules coupled with electrically-gated PL measurements to demonstrate direct signatures of MoS_2 functionalization, detected using the defect-related excitonic peak in low temperature PL of MoS_2 [2].

References:

- [1] K. Greben, *et al.*, arXiv: **2009.12808**, (2020).
- [2] K. Greben, S. Arora, M. G. Harats, and K. I. Bolotin, Nano Lett **20**, 4 (2020).



Personal Information:

Name: Samuel Palato

Project: B9

Office number: (030) 8413-5130

e-mail: palato@fhi-berlin.mpg.de

Time-resolved interferometric nanoscopy

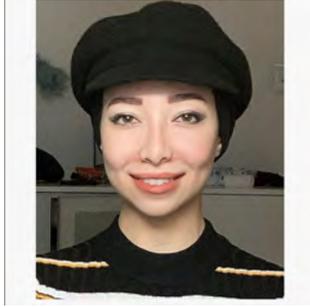
Samuel Palato

Abstract:

The electronic properties of TMDC monolayers are strongly influenced by their local dielectric environment. The optical properties of these materials thus exhibit spatial variations in the vicinity of domain edges and structural defects [1]. These modifications to the energy levels extend over tens to hundreds of nm, a length scale below the diffraction limit. The study of spatial dependence of electronic processes calls for the development of an experimental tool capable of probing the electronic response with nanometer resolution on femtosecond timescales: time-resolved interferometric nanoscopy (TRION). This technique exploits the near-field enhancement in the vicinity of a metallic nanotip to obtain nanometer resolution, and femtosecond laser pulses in a pump-probe scheme to obtain femtosecond resolution. The method is capable of measuring the complex dielectric response of the material, thus revealing local variations in electronic energy and dynamics [2]. The experimental challenges to the realization of TRION in the visible regime are presented. Preliminary results on WS₂ monolayers reveal variations of the electronic response on sub-micron length scales around defect and edges. The prevalence of different defect types depends on the synthesis technique. The development of TRION will enable unprecedented insights into the spatiotemporal dynamics of electronic excitations in TMDCs and heterostructures.

References:

- [1] W. Bao, *et al.*, Nat. Commun. **6**, 7993 (2015).
- [2] M. A. Huber, *et al.*, Nat. Nano. **12**, 207 (2017).

**Personal Information:****Name:** Alaa Akkoush**Project:** A13**Office number:** (030) 8413 4855**e-mail:** akkoush@fhi-berlin.mpg.de

Benchmarking electric field responses in FHI-aims

Alaa Akkoush, Christian Carbogno and Mariana Rossi

Abstract:

Polarization is an essential property of materials that is linked to diverse experimental observables such as born effective charges, dielectric constant and piezoelectric coefficients, in addition to Raman and infrared intensities [1]. In this work, we describe the implementation of polarization and its response to electric fields within the FHI-aims code [2]. This code is an all electron full potential ab-initio molecular simulations code based on numerically tabulated atom-centered orbitals (NAOs) [3]. Afterwards, we present examples related to the response of polarization with respect to atomic displacements and applied electric fields in two showcase applications. The first application relates to the evaluation of Born effective charges throughout the direct to indirect band-gap transition in the layered transition metal dichalcogenide material MoS₂. The second application involves model simulations of enhanced Raman spectra obtained from local electronic-density responses of organic molecules on inorganic surfaces.

References:

- [1] J. B. Neaton, *et al.*, Phys. Rev. B. **71**, 014113 (2005).
- [2] H. Shang, *et al.*, New J. Phys **20**, 073040 (2018).
- [3] V. Blum, *et al.*, Comp. Phys. Comm. **180**, 2175–219 (2009).

**Personal Information:****Name:** Jannis Krumland**Project:** B16**Office number:** (030) 2093-66411**e-mail:** krumlanj@physik.hu-berlin.de

First-principles simulations of excitation dynamics in organic systems under realistic conditions

Jannis Krumland, Ana M. Valencia and Caterina Cocchi

Abstract:

Recently, the importance of vibronic coupling in the ultrafast dynamics following a photoexcitation in materials has become more and more appreciated, e.g. in the context of optoelectronics and photovoltaics. Gaining a deeper understanding of these processes is paramount to fully exploit their technological potential. We demonstrate that real-time time-dependent density functional theory, coupled to the Ehrenfest scheme for classical molecular dynamics, offers an insightful description of the excitation dynamics in light-absorbing systems. The ultrafast pulse is explicitly included as a time-dependent external field, while solvents and substrates are modeled implicitly as polarizable continua. Considering ethylene, thiophene, and benzene molecules as building blocks of complex molecular systems, we demonstrate and rationalize the strong interplay between electronic excitations and vibrational modes. The results obtained in these compounds confirm the prominent role of vibronic coupling in the ultrafast dynamics of molecules, also coupled to inorganic substrates [1].

References:

- [1] J. Krumland, A.M. Valencia, S. Pittalis, C.A. Rozzi, C. Cocchi, to be submitted , (2020).

**Personal Information:****Name:** Olga Turkina**Project:** B11**Office number:** (030) 2093 66386**e-mail:** turkina@physik.hu-berlin.de

Charge-transfer excitons at the n P-pyridine/ZnO(10 $\bar{1}$ 0) ($n = 0, 1, 2$) hybrid interface

Olga Turkina, Dmitrii Nabok, Andris Gulans, Caterina Cocchi, and Claudia Draxl

Abstract:

By combining all-electron density-functional theory with many-body perturbation theory, we investigate three prototypical inorganic/organic hybrid systems, composed of either pyridine [1], 1P- or 2P-pyridine molecules that are chemisorbed on the non-polar ZnO(10 $\bar{1}$ 0) surface. We employ the G_0W_0 approximation to describe its one-particle excitations in terms of the quasi-particle band structure, and solve the Bethe-Salpeter equation for obtaining the absorption spectrum. We explore the nature of the optical excitations at the interface for each system over a wide energy range and show that various kinds of electron-hole pairs are formed, comprising hybrid excitons and (hybrid) charge-transfer excitations. For selected examples of either exciton type, we analyze the individual contributions from the valence and conduction bands and discuss the binding strength and extension of the electron-hole wavefunctions. As we change the inorganic component from pyridine to 1P- and 2P-pyridine by adding phenyl rings, we observe the following trends: (hybrid) charge-transfer excitons appear at progressively lower energies due to shrinking of the molecular band gap and become more hybrid as more bands with diverse character are involved in their formation.

References:

- [1] O. Turkina, *et al.*, Adv. Theory Simul. **2**, 1800108 (2019).



Personal Information:

Name: Dominik Christiansen

Project: B12

Office number: 030 314 27658

e-mail: dominik.christiansen@tu-berlin.de

Theory of time-resolved ARPES on monolayer transition-metal dichalcogenides

Dominik Christiansen, Malte Selig, Ermin Malic, Ralph Ernstorfer and Andreas Knorr

Abstract:

Time and angle resolved photoemission spectroscopy (tr-ARPES) allows to investigate the ultrafast dynamics of electronic excitations directly in momentum space [1]. However, materials such as monolayer transition-metal dichalcogenides (TMDC) or hybrid interfaces of different materials exhibit tightly bound excitons, which dominate their optical properties. The variety of optically bright and dark exciton states has a crucial impact on the exciton lifetime and relaxation dynamics [2].

Here, we develop an excitonic theory of time-resolved ARPES, showing that tr-ARPES is able to directly access excitons and probe their dynamics throughout the Brillouin zone [3]. We discuss the extension of our theory to functionalized TMDCs where a more complex exciton dynamics take place due to spatial energy or charge transfer [4,5].

References:

- [1] M. Puppini, *et al.*, Rev. Sci. Instrum. **90**, 023104 (2019).
- [2] M. Selig, *et al.*, 2D Mater. **5**, 035017 (2018).
- [3] D. Christiansen, *et al.*, Phys. Rev. B **100**, 205401 (2019).
- [4] J.F. Specht, *et al.*, Phys. Rev. Appl. **9**, 044025 (2018).
- [5] M. Selig, *et al.*, Phys. Rev. B **99**, 035420 (2019).



Personal Information:

Name: Hélène Seiler

Project: B17

Office number: (0)30 8413-5134

e-mail: seiler@fhi-berlin.mpg.de

Structural dynamics of pentacene single crystals and MoS₂/pentacene heterostructures

Hélène Seiler, Marcin Krynski, Daniela Zahn, Benedikt Haas, Johannes Müller, Xiaomin Xu, Soohyung Park, Thomas Vasileiadis, Yoav W. Windsor, Yingpeng Qi, Sebastian Hammer, Jens Pflaum, Norbert Koch, Christoph T. Koch, Mariana Rossi, Heinrich Schwörer and Ralph Ernstorfer

Abstract:

Singlet fission has attracted significant attention for its relevance in photovoltaics. It is known that the static crystalline structure strongly impacts singlet fission properties, and the structural dynamics is thought to play an essential role in the spatial separation of the triplets. Yet to this day, a direct probe of the molecular motions involved in a singlet fission process has been lacking. Here we directly observe the structural dynamics accompanying the singlet fission process in single crystal pentacene using femtosecond electron diffraction (FED). Our data reveal the presence of incoherent structural dynamics, as well as coherent atomic motions at 1 THz. Molecular dynamics simulations enable us to attribute these coherent motions to collective inter-molecular motions involving several molecules and featuring high dynamical heterogeneity. By moving entire molecules against each other, these motions transiently modify the transfer integral between orbitals of different molecules, which may modulate the singlet fission rate. The physical insights gained from the single crystal pentacene samples will be exploited to interpret FED data on a MoS₂/pentacene heterostructure, with the ultimate aim of revealing the dynamics of interfacial vibrational energy transfer.



Personal Information:

Name: Günter Kewes

Project: B18

Office number: (0)30 2093-7798

e-mail: gkewesatphysik.hu-berlin.de

Extreme light-matter interaction with plasmonic nanoantennas

Günter Kewes, Felix Stete, Wouter Koopman, Nils Bochow and Oliver Benson

Abstract:

The research field of plasmonics is driven by the hope to boost the strength of light-matter interaction with intense near-fields and to increase the integration density of optical-electronic elements. Actual applications have mostly been limited by the intrinsic properties of the used metal nanostructures, i.e., luminescence quenching, absorption losses and heat production. However, in recent years fascinating results have been reported in plasmonics, namely strong coupling with fluorophores at ambient conditions as well as electrically driven light emission by inelastic tunneling. Both processes become possible/efficient, when extreme hotspots are spatially matched with fluorophores/electrical currents. Here we report on our current attempts to understand and model such systems and to establish a reproducible production and quick characterization of quasi identical nanoparticle on mirror (NPoM) antennas in the lab. Our current results indicate that the description of fluorophores with the dipole approximation fails in such systems, i.e., complete exciton wavefunctions must be taken into account.



Personal Information:

Name: Dan-Nha Huynh

Project: B10

Office number: (030) 2093 - 4934

e-mail: dhuynh@physik.hu-berlin.de

Different approaches to the hydrodynamic material model within the discontinuous Galerkin time-domain method

Dan-Nha Huynh, Francesco Intravaia and Kurt Busch

Abstract:

One popular way to describe plasmonic nano-structures is the hydrodynamic material model – a nonlinear as well as nonlocal model. To analyze the associated nonlinear effects we find a perturbative approach to the hydrodynamic model to be beneficial as we cannot only clearly separate linear and nonlinear spectra but also display time-resolved nonlinear field information. To this end, we integrate the material model into a numerical discontinuous Galerkin time-domain scheme [1], where the perturbative hydrodynamic material equations are solved alongside with Maxwell’s equations. The resulting numerical scheme is demonstrated on a silver nano-wire setup, where we perform three-wave-mixing with two ultra-short excitation pulses. Thereby, we use the setup’s resonances to tune the incoming pulses’ center frequencies so that the optimal nonlinear output intensity is achieved [2].

As a second approach to the hydrodynamic model we focus on its linearized version but now extend the linear model by introducing an additional drift current density. The result is a hybrid between the original hydrodynamic model for metals and the drift-diffusion model for semi-conductors. We offer some preliminary results on this novel material model.

References:

- [1] K. Busch, M. König, and J. Niegemann, *Laser & Photonics Reviews* **5**, 773 (2011).
- [2] D. Huynh, *et al.*, *Applied Physics B* **122**, 1 (2016).



Personal Information:

Name: Maurizio Roczen

Project: Z3

Office number: (030) 2093 66374

e-mail: sfb951@physik.hu-berlin.de

Family and career support during the COVID-19 pandemic

Maurizio Roczen

Abstract:

Ensuring a family-friendly work environment and supporting the career of our staff are both of major importance for the CRC 951. In order to provide the best possible working conditions for all our staff -especially during the current COVID-19 pandemic- we offer a wide range of services and measures, such as mobile and flexible childcare services, support in finding free Kita spots, coaching workshops, establishment of home offices, and much more.

This talk will give you an overview of our versatile programs to provide family friendliness as well as career support and how to apply for our programs.



Personal Information:

Name: Patrick Amsalem

Project: A8

Office number: (030) 20937553

e-mail: Amsalem@physik.hu-berlin.de

Substrate-dependent charge transfer mechanisms between monolayer MoS₂ and molecular dopants

Patrick Amsalem, Soohyung Park, Thorsten Schultz, Xiaomin Xu, Berthold Wegner, Areej Aljarb, Ali Han, Lain-Jong Li, Vincent C . Tung and Norbert Koch

Abstract:

2D transition metal dichalcogenides monolayer films have recently gained enormous attention. Yet, to extend the range of applications of these emerging materials, tuning their Fermi level is of crucial importance. Here, we report on the adsorption of a strong p-type organic dopant, 3,4,5,7,8-hexafluoro-tetracyanonaphthoquinodimethane (F₆TCNNQ), as a possibly efficient route for Fermi-level tuning of MoS₂[1]. More specifically, we employ angle-resolved UV and X-ray photoelectron spectroscopy to reveal the charge transfer (CT) mechanisms taking place at the MoS₂/organic interface as a function of the electrical properties of the supporting substrates, which are here chosen to be sapphire, graphite and gold. Interestingly, the CT mechanisms are found to strongly differ as a function of the substrates, which results in markedly contrasted doping efficiencies. The reported findings can be exploited for the design of advanced hybrid heterostructures with tailored electronic properties.

References:

- [1] S. Park *et al.*, Communications. Physics **2**, 109 (2019).



Personal Information:

Name: Sven Lubeck

Project: B11

Office number: 030209366450

e-mail: lubeck@physik.hu-berlin.de

Spin-orbit interaction in first-principles calculations of transition metal dichalcogenides

Sven Lubeck

Abstract:

Producing quantitative results from first-principles calculations of realistic hybrid inorganic/organic systems (HIOS) is a challenging task for solid-state theory. Depending on the material and property of interest, calculations can be made feasible by applying a variety of approximations, such as neglecting crystallographic defects, the finite size of the system, temperature, and relativistic effects. When studying HIOS that incorporate transition metal dichalcogenides (TMDCs), relativistic effects like spin-orbit interaction should not be neglected since they affect the electronic structure considerably [1]. For this reason, an efficient method that sufficiently accounts for spin-orbit effects is desirable.

In this presentation, I will introduce three different approaches to including spin-orbit interactions in density-functional-theory and *GW* calculations. I will demonstrate their respective capabilities by presenting computed properties of the four TMDC monolayers MoS₂, MoSe₂, WS₂, and WSe₂. Studying their performance with respect to accuracy and computational cost will reveal the optimal approach for the application to TMDC-based HIOS.

References:

- [1] Z. Y. Zhu, Y. C. Cheng, and U. Schwingenschlögl, Phys. Rev. B **84**, 153402 (2011).



Personal Information:

Name: Cecilia Vona

Project: B 11

Office number: 66370

e-mail: cvona@physik.hu-berlin.de

Electronic structure of (organic)-inorganic metal halide perovskites: the dilemma of choosing the right functional

Cecilia Vona, Dmitrii Nabok and Claudia Draxl

Abstract:

Organic-inorganic metal halide perovskites (HaPs) are materials widely studied for their light-harvesting properties. Owing to the interplay between strong electron-electron interaction and spin-orbit coupling, their theoretical investigation is still a challenge. Here we evaluate methodologies to compute the electronic structure of APbI_3 , where A can be organic like MA or FA, or inorganic like Cs, and their precursor PbI_2 . To this extend, we investigate several approaches within density functional theory (DFT) and many-body perturbation theory (MBPT), taking into account spin-orbit coupling effects. Hybrid functionals, such as PBE0 and HSE, are at the center of the investigation, since they can provide results as accurate as MBPT at a lower computational cost. Hence, we explore several methods to tune the parameters of the hybrid functionals. Additionally, at the MBPT level, we investigate the dependence of the calculations from the DFT starting point. All the calculations are performed with the full-potential all-electron computer package `exciting`, which employs LAPW+lo basis sets. We observe that hybrid functionals with a proper α value are the most suitable to compute the electronic structure of APbI_3 .



Personal Information:

Name: Giovanni Procida

Project: B16

Office number: +49 441 798 3552

e-mail: giovanni.procida@uol.de

Optical properties and structure-property relations of lead halide perovskite building blocks in solution

Giovanni Procida, Richard Schier, Ana M. Valencia and Caterina Cocchi

Abstract:

Reaching certified power conversion efficiency on small areas, hybrid metal-halide perovskites are the best solution-processed solar cells that are currently available. Despite rapid development, there are still many questions unanswered regarding the fundamental characteristics of these materials. Characterizing the optical properties of metal-halide perovskite building blocks in different solution environments is of great relevance to link the nature and quantity of precursors to the final optoelectronic properties. For this purpose, we adopt the first-principles framework of time dependent density functional theory [1] coupled to the polarizable continuum model [2,3] to unravel the optical properties of molecular precursors of lead halide perovskites. We analyze the effects of different solvent molecules by treating them atomistically as well as implicitly in order to address the specific molecular interactions between the iodoplumbate complexes and the solvent molecules.

References:

- [1] E. Runge, E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984).
- [2] M. J. Frisch.; *et al.*, Gaussian 16, Revision A.03; Gaussian, Inc.: , Wallingford,CT, USA, (2016).
- [3] J. Tomasi, B. Mennucci, and R. Cammi, Chem. Rev. **105**, 2999–3094 (2005).

Poster Session

The Poster Session starts on Wednesday, 18th November 2020, at 01:00 pm.

General Information

After entering the ZOOM room, you will be able to activate your microphone and camera. Poster presenters are asked to keep both activated at all times. The posters will be presented in different breakout rooms, numbered according to the poster numbers. To visit another poster, please leave the room you are currently in by clicking on the button "Leave breakout room" in the lower right corner of the ZOOM window. You will be able to choose between leaving the breakout room or leaving the entire meeting.



Personal Information:

Name: Alberto Eljarrat

Project: Z2

Office number: (030) 2093-7734

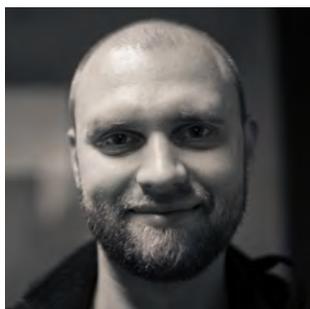
e-mail: aeljarrat@physik.hu-berlin.de

Studying SPR mode dispersion and temporal coherence in dye-embedded silica-covered Ag-NWs

Alberto Eljarrat, Martin Rothe, Günter Kewes, Oliver Benson, Yuhang Zhao, Yan Lu and Christoph T. Koch

Abstract:

Electron energy-loss spectroscopy (EELS) in the recently installed Nion high-resolution monochromated EELS-STEM (HERMES) instrument opens new possibilities for the analysis of hybrid inorganic/organic systems. We present detailed results obtained from the observation of J-aggregate dye embedded silica-covered silver nano-wire (NW) samples. Using spectrum-imaging acquisitions, in which each pixel contains an EELS spectrum, and specialized software developed in-house, EELS reveals the energy and spatial distribution of surface plasmon resonance (SPR) modes. Using a new automatic technique, we have also been able to retrieve the dispersion relations, $\omega = \omega(k)$, for these structures. This information entails dampening of the different SPR modes with respect to the presence of the J-aggregate dye molecules and silica-cover. Moreover, traces of the J-aggregate are found in the spectra, hinting the possibility of direct detection of these molecules. The STEM-EELS technique proves specially suited for these tasks given the great spatial and energy resolution, at the nm and meV level, respectively, and we demonstrate this in acquisitions covering a μm sized field of view. We are also studying novel capabilities, using Fourier transformation of our spectra to reveal information about the dynamics of the SPR mode response. This technique obtains a fs-resolution movie of the SPR coherence, allowing the direct observation of the return-time over several cycles.

**Personal Information:****Name:** Dmitrii Maksimov**Project:** A 13**Office number:** +4917675197703**e-mail:** maksimov@fhi-berlin.mpg.de

Ab initio structure search of (flexible) molecules at interfaces

Dmitrii Maksimov, Haiyuan Wang and Mariana Rossi

Abstract:

Searching for stable structures of molecular adsorbates (in isolation or forming layers) becomes challenging especially for weakly bonded systems or when the adsorbates are flexible. In order to make this problem tractable with ab initio potentials, we developed a random structure search package that takes explicitly into account the flexibility of molecules and their position with respect to fixed surroundings. We couple this search strategy with an efficient structure optimization algorithm, making use of geometry optimizer preconditioners that are especially tailored to accelerate the optimization of van der Waals bonded structures and that can handle large structure changes. We show performance gains in ab initio geometry optimization with these techniques, and prediction of structure of molecules adsorbed on TMDC monolayers.



Personal Information:

Name: Dragos Mutruc

Project: A3

Office number: 2093-7453

e-mail: dragos.mutruc@hu-berlin.de

Modulating Guest Uptake in Core-Shell MOFs with Visible Light

Dragos Mutruc, Alexis Goulet-Hanssens, Sam Fairman, Sebastian Wahl, Christopher Knie, Annett Zimathies and Stefan Hecht

Abstract:

Functional materials that are able to adapt their structure in response to external stimuli have gained increased attention in applications as “smart” materials. Light is the most attractive among these stimuli as it is tunable in wavelength and intensity, provides unparalleled spatio-temporal resolution, is non-invasive and can be applied remotely. Metal-organic frameworks (MOFs) are a promising class of crystalline, porous solids with exceptionally high accessible internal surface areas, consisting of metal nodes or clusters connected with organic linker molecules. Recent examples have shown that incorporating molecular switches, namely azobenzenes, is a viable strategy to obtain light-responsive MOFs. Here, we report on the synthesis and characterization of a two-component core-shell MOF with a large and porous interior for guest storage covered by a thin photoswitchable outer shell, which functions as a light-controlled barrier for uptake and release of guest molecules. Our linker design was motivated by the concept of a light-responsive MOF with large pores gated by large photoswitchable “doors”. Molecular guest uptake and release experiments show a significant difference between the E- and Z-states, confirming the photoinduced change of the pore window size in the shell. [1]

References:

- [1] D. Mutruc, *et al.*, *Angew. Chem. Int. Ed.* **58**, 12862 (2019).



Personal Information:

Name: Hu Lin

Project: A6

Office number: +4915908699481

e-mail: linhu621@physik.hu-berlin.de

Reversible Switching of Charge Transfer at the Graphene–Mica Interface with Intercalating Molecules

Hu Lin, José D. Cojal González, Nikolai Severin, Igor M. Sokolov and Jürgen P. Rabe

Abstract:

Understanding and controlling charge transfer through molecular nanostructures at interfaces is of paramount importance, particularly for electronic devices but also for contact electrification or in bio-electronics. We demonstrate here reversible switching of charge transfer at graphene-mica interface by molecularly thin layers of fluid molecules intercalating the interface. While water intercalating the interface blocks charge transfer [1], organic molecules like ethanol filling initially dry interface, or diffusively replacing water do not block or restore the charge transfer at the interface respectively. We propose a charge transfer model between occupied mica trap states and electronic states of graphene, offset by the electrostatic potentials produced by the molecular dipole layers, as supported by molecular dynamics simulations. Our work facilitates the understanding of the influence of molecular intercalants onto charge transfer at interfaces.

References:

- [1] H. Lin, A. Schilo, A. R. Kamoka, N. Severin, *et al.*, Phys. Rev. B **95**, 195414 (2017).



Personal Information:

Name: Ignacio Gonzalez Oliva

Project: B11

Office number: (030) 2093-66368

e-mail: gonzalez@physik.hu-berlin.de

Electron-phonon coupling in hybrid inorganic/organic systems: implementation within the LAPW formalism

Ignacio Gonzalez Oliva, Fabio Caruso and Claudia Draxl

Abstract:

Electron-phonon interactions (EPI) are ubiquitous in condensed matter and manifest themselves in a wide range of physical phenomena [1]. However, due to their high computational cost EPI calculations are mostly restricted to systems with a few atoms per unit cell [2]. We are developing an effective first-principles approach to extend EPI calculations to hybrid inorganic/organic systems (HIOS). Considering the vibrational properties of the constituents, we include their effects in the electronic properties of the hybrid system. To this extent we employ density-functional theory (DFT) where the Kohn-Sham (KS) eigenvalues and eigenvectors provide a starting point for subsequent calculations of the electron-phonon self energy. This approach is being implemented in the `exciting` code, a full-potential all-electron code based on the linearized augmented plane-wave plus local orbitals (LAPW + lo) method [3]. We will present details on the implementation, comparison between the frozen-phonon method and density-functional perturbation theory and preliminary results on hybrid systems consisting of a molecule on top of monolayer MoS₂.

References:

- [1] F. Giustino, *Rev. Mod. Phys.* **89**, 015003 (2017).
- [2] C. Draxl, D. Nabok, and K. Hannewald, *Acc. Chem. Res.* **47**, 3225 (2014).
- [3] A. Gulans *et al.*, *J. Phys. Condens. Matter* **26**, 363202 (2014).



Personal Information:

Name: Kristin Klaue

Project: A3

Office number: +49 (0)30 2093-7453

e-mail: kristin.klaue@hu-berlin.de

Donor–Acceptor Dihydropyrenes Switchable with Near-Infrared Light

Kristin Klaue, Wenjie Han, Pauline Liesfeld, Fabian Berger, Yves Garmshausen and Stefan Hecht

Abstract:

The incorporation of photochromic moieties in complex molecular systems enables a wide variety of applications in materials and life sciences. For most of these applications, visible or near-infrared (NIR) light is more suitable than UV light due to its greater penetration depth and non-damaging character. However, the isomerization of photoswitches usually requires high-energy photons in at least one direction. One class of photoswitches, which can be operated with visible light are dihydropyrenes (DHPs), pioneered by Boekelheide and Mitchell. [1]

Here we show a general design strategy for direct one-photon NIR photoswitches based on strong donor-acceptor DHPs, which display strongly bathochromic charge-transfer bands and exhibit a pronounced positive solvatochromism. In the closed DHP isomers, the donor and acceptor substituents are π -conjugated and hence the DHPs exhibit a partial quinoid character, giving rise to a long-wavelength transition depending on the donor-acceptor strength. Upon photo-induced ring-opening with far-red or NIR light the cross-conjugated cyclophanediene (CPD) isomer is formed, which in turn decouples the donor and acceptor substituents. The thermal half-lives of the metastable CPDs range from milliseconds to hours depending on the polarity of the environment. The use of these donor-acceptor DHPs allows efficient photoswitching induced by NIR light, which renders them attractive for various applications. [2]

References:

- [1] R. H. Mitchell, *Eur. J. Org. Chem.*, 2695 (1999).
- [2] K. Klaue, *et al.*, *J. Am. Chem. Soc.* **142**, 11857 (2020).



Personal Information:

Name: Manuel Katzer

Project: B12

Office number: 030-314-23764

e-mail: manuel.katzer@physik.tu-berlin.de

Charge And Energy Transfer in Bilayer TMDCs and Hybrid Molecule-TMDC Structures

Manuel Katzer, Andreas Knorr and Malte Selig

Abstract:

At the interfaces of van der Waals heterostructures, different forms of energy and charge transfer occur, including Förster- and Dexter-type transitions as well as tunneling processes [1]. Those phenomena are of fundamental interest as they offer a plethora of new opportunities for technical applications [2]. Here, we develop a Heisenberg equations of motion theory [3,4] for the interlayer relaxation of optical excitations in vdW heterostructures. In a second step, this approach will be generalized to hybrid inorganic/organic structures of molecule-TMDC compounds, which are currently intensively studied experimentally [5]. We work towards proposing an accessible platform for the realisation of multiexcitation bound states, as they occur e.g. in boson impurity models [6].

References:

- [1] G. Froehlicher, E. Lorchat, and S. Berciaud, Phys. Rev. X **8**, 011007 (2018).
- [2] W. Yu, Y. Liu, H. Zhou, A. Yin, Z. Li, Y. Huang and X. Duan, Nature Nanotech **8**, 952–958 (2013).
- [3] M. Selig, E. Malic, K.J. Ahn, N. Koch, and A. Knorr, Phys. Rev. B **99**, 035420 (2019).
- [4] S. Ovesen, S. Brem, C. Linderålv, M. Kuisma, T. Korn, P. Erhart, M. Selig, and E. Malic, Commun Phys **2**, 23 (2019).
- [5] G. Reecht, N. Krane, C. Lotze, and K. J. Franke, ACS Nano **13**, (6) 7031-7035 (2019).
- [6] T. Shi, Y. Wu, A. González-Tudela, and J.I. Cirac, Phys. Rev. X **6**, 021027 (2016).

**Personal Information:****Name:** Marcel Schloz**Project:** A12/Z2**Office number:** 030 20930 7734**e-mail:** schlozma@hu-berlin.de

Overcoming information reduced data and experimentally uncertain parameters in ptychography with regularized optimization

Marcel Schloz, Thomas C. Pekin, Wouter Van den Broek and Christoph T. Koch

Abstract:

Reconstruction algorithms play a crucial role in the coherent diffractive imaging method called ptychography. To ensure a high quality reconstruction and thus the practical applicability of this method, the algorithm does not only have to retrieve an image of a specimen from a series of diffraction patterns, it is also required to cope with data that may have been acquired with non ideal hardware or under non ideal experimental conditions. Situations, where for example the illuminating probe is distorted or suffering from incoherence, the scanning positions are imprecise and the data is degraded by noise, are in fact abundant. While progress in the development and improvement of reconstruction algorithms enabled to tackle these issues [1-4], a success is not necessarily guaranteed. Especially in cases where the data is low in information, reconstruction algorithms tend to fail. One approach that not only improves the quality of the ptychographic reconstruction in general, but also allows the algorithm to successfully converge in these extreme cases, is based on the inclusion of prior information to the optimization [5]. Here, we demonstrate the beneficial effect of prior information on the method ptychography.

References:

- [1] P. Thibault, *et al.*, *Ultramicroscopy* **109.4**, 338 (2009).
- [2] A. Maiden, *et al.*, *Ultramicroscopy* **120**, 64 (2012).
- [3] V. Katkovnik, *et al.*, *JOSA A* **30.3**, 367 (2013).
- [4] A. Maiden, *et al.*, *Optica* **4.7**, 736 (2017).
- [5] M. Schloz, *et al.*, *Opt. Express* **28**, 28306 (2020).



Personal Information:

Name: Martin Rothe

Project: B2

Office number: (030) 2093-4934

e-mail: rothe@physik.hu-berlin.de

Local-chirality sensors for HIOS from self-assembled plasmonic nano-antenna-waveguide structures

Martin Rothe, Yuhang Zhao, Johannes Müller, Siavash Qodratipour, Günter Kewes, Christoph Koch, Yan Lu and Oliver Benson

Abstract:

The chirality of an object is the property, that it can not be superimposed with its mirror image. The occurrence of different structures and orientations in HIOS on a very microscopic scale, can manifest as structural chirality, but is difficult to investigate by optical methods. We developed a symmetry-broken plasmonic nano-antenna-waveguide structure with encapsulated modified PDI molecules based on our Silica-coated Silver nanowires[1]. We have measured how inside this nanoscopic structure, the circular polarization of an incident light field is translated into fluorescence of the PDI at defined spatial positions via chiral coupling. Guided by numerical simulations, we show how the circular polarization of the light field is transformed into a chirality of the plasmonic near-field[2]. The formation of a chiral hot-spot suggests the desired sensing application for HIOS with optical near-field resolution far below the diffraction limit. On our poster, we will also show the recent experimental results on the implementation of a functional magnetic antenna into this system. Fourier analysis of the time-evolution of the emission signal under a varying magnetic field gives us both, active control about and simultaneous insight into the occurrence of plasmonic chiral near-fields.

References:

- [1] M. Rothe, Y. Zhao, G. Kewes, Z. Kochovski, W. Sigle, P. A. van Aken, C. Koch, M. Ballauff, Y. Lu, and O. Benson, *Sci Rep* **9**, 3859 (2019).
- [2] M. Rothe, Y. Zhao, J. Müller, G. Kewes, C. Koch, Y. Lu, and O. Benson, , submitted (2020).



Personal Information:

Name: Matheus Jacobs

Project: B16

Office number: 030 2093 66411

e-mail: jacobs@physik.hu-berlin.de

Ultrafast charge transfer and vibronic coupling in donor/acceptor interfaces from first principles

Matheus Jacobs, Jannis Krumland, Ana M. Valencia and Caterina Cocchi

Abstract:

Donor-acceptor (DA) interfaces are ubiquitous materials for opto-electronic applications and strongly characterize their intrinsic properties. Interfacial charge transfer in particular, plays a crucial role in the electronic structure and optical response of these systems. For this reason, it is essential to gain microscopic insight on the fundamental processes involved at the interface also beyond the static picture. In the framework of real-time time-dependent density-functional theory coupled to Ehrenfest molecular dynamics, we investigate the microscopic mechanisms driving ultrafast charge transfer at DA interfaces. Specifically, we address the role of vibronic coupling in systems perturbed by an external laser pulse. For this purpose, we analyze the inorganic/organic interface formed by the acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyano-quinodimethane (F4TCNQ) adsorbed on a hydrogenated silicon cluster. We demonstrate that the nature and amount of charge transfer in these systems results from a complex interplay between coupled electronic and vibrational degrees excited by the laser pulse [1].

References:

- [1] M. Jacobs, *et al.*, submitted to *Advances in Physics: X*, (2019).



Personal Information:

Name: Meysam Raoufi

Project: B7

Office number: 331-977-5633

e-mail: raoufi@uni-potsdam.de

Probing the charge carrier dynamics in hybrid layer stacks comprising a TMDC monolayer and an organic semiconductor

Meysam Raoufi, Sreelakshmi Chandrabose, Toni Haubitz, Nicolas Zorn Morales, Niklas Mutz, Michael Kumke, Sylke Blumstengel and Dieter Neher

Abstract:

Two-dimensional transition metal chalcogenides (TMDCs) exhibit excellent optical properties. This motivates recent efforts to combine TMDCs with organic semiconductors. Recently, reasonable photovoltaic performance was demonstrated for hybrid TMDC/Organic semiconductor devices [1, 2]. Here, we present results on the optical properties of monolayers of TMDCs interfaced with an organic hole transport material. By performing steady state photoluminescence (PL) and ultrafast transient absorption spectroscopy (TAS) on the neat TMDC and the hybrid TMDC/organic stack, we resolve ultrafast exciton dissociation and charge carrier dynamics at the hybrid interface. For MoS₂ combined with the hole transport molecule α -NPD, we find that the dynamics of the TMDC excitons is largely governed by the trapping and recombination of charges on the MoS₂ layer, while we also resolve a long-lived signal which we assign to charge separation. In line with recent experiments on MoS₂/Pc hybrid systems [3], we explain the relatively low efficiency of charge transfer to the weak electronic coupling between the two components. These results serve as guidance for the optimization of the hybrid layer stack towards the goal to realize efficient TMDC exciton dissociation into hybrid charge transfer states and finally into free charges.

References:

- [1] T. A. Shastry, *et al.*, ACS nano **10**, 10573 (2016).
- [2] T. R. Kae, *et al.*, ACS nano **17**, 164 (2017).
- [3] S. Padgaonkar, *et al.*, Phys.Chem. C **123**, 13337 (2019).



Personal Information:

Name: Nicolas Zorn Morales

Project: B14

Office number: (030) 2093-7546

e-mail: nicolas.zorn.morales@hu-berlin.de

Switching impact of photochromic diarylethenes as self-assembled monolayers in organic light emitting diodes

Nicolas Zorn Morales, Giovanni Ligorio, Qiankun Wang, Giovanni Cotella, Björn Kobin, Franco Cacialli, Stefan Hecht, Norbert Koch and Emil List-Kratochvil

Abstract:

Self-assembled monolayers (SAMs) have proven their capability for improving organic electronic device performance by adjusting the energy-level alignment at hybrid inorganic/organic interfaces. Beside the enhancement of device performance, the fabrication of multifunctional devices in which the output can be modulated by multiple external stimuli remains a challenging target.

Here we report on the functionalization of a transparent electrode such as indium tin oxide (ITO) with SAM realized with a derivative of a switching molecule (diarylethene) enabling optical control of electronic properties over the ITO interface. By combining a range of surface characterization such as contact angle, scanning force microscopy photoemission spectroscopy, we present a detailed picture of the SAM binding onto ITO. As a proof-of-principle, an organic lightemitting diode embedding the SAM-covered electrode was fabricated and characterized. The illumination of the two terminal device with defined external wavelengths enables reversible control on the device luminescence. This expanded functionality is based on the photoinduced modulation of the electronic structure of the diarylethene isomers, which impact the charge carriers confinement within the emissive layer. This approach could be exploited for the realization of novel opto-electronic logic circuits, that can be externally controlled by light.



Personal Information:

Name: Pauline Liesfeld

Project: A3

Office number: (030) 2093-7508

e-mail: liesfelp@chemie.hu-berlin.de

Highly Cooperative Photoswitching in Dihydropyrene Dimers

Pauline Liesfeld, Yves Garmshausen, Simon Budzak, Jonas Becker, Andre Dallmann, Denis Jacquemin and Stefan Hecht

Abstract:

For systems composed of multiple photochromic units the coupling of the individual switching events is hard to predict and the bridging moiety has shown to be a crucial factor. Typically, the loss of photochromism or diminished quantum yields are observed for the second switching event.[1] In contrast dihydropyrenes, pioneered by Mitchell and Boekelheide, are negative T-type photoswitches exhibiting great potential for the use in multiphotochromic systems.[2,3]

We present symmetrical bis-photochromes consisting of two dihydropyrenes conjugated either through a suitable acceptor or donor bridge, resulting in three accessible states (closed-closed vs. closed-open vs. open-open). In some derivatives we have been able to uncover a cooperative switching behavior in which the second ring-opening event is 100 times more efficient than the first one.[4] Based on our insights into the mechanism of information transfer we aim to design multiphotochromic systems with enhanced switching efficiencies.

References:

- [1] A. Fihey, A. Perrier, W. Browne, D. Jacquemin, *Chem. Soc. Rev.* **44**, 3719 (2015).
- [2] R. Mitchell, V. Boekelheide, *J. Am. Chem. Soc.* **92**, 3510 (1970).
- [3] R. Mitchell, *et al.*, *J. Org. Chem.* **71**, 327 (2006).
- [4] P. Liesfeld, *et al.*, *Angew. Chem. Int. Ed.* **59**, 19352 (2020).



Personal Information:

Name: Raymond Amador

Project: B16

Office number: (030) 2093 66411

e-mail: raymonda@physik.hu-berlin.de

Electronic and optical properties of Na_2KSb and NaK_2Sb from ab initio many-body theory

Raymond Amador, Caterina Cocchi and Bob Smith

Abstract:

Multi-alkali antimonides have drawn particular interest in the last few years as novel materials for electron sources. Among them, sodium-potassium-antimonides are regarded as especially promising for their band gaps in the infrared/visible region. Our first-principles study utilises the framework of density-functional theory and manybody perturbation theory to calculate the electronic and optical properties of Na_2KSb and NaK_2Sb . This approach has already been successfully adopted in conjunction with experiments to shed light on the intrinsic properties of Cs-based alkali antimonides [1-2]. The analysis of band structures and densities of state indicate that both materials are characterised by a direct quasi-particle gap on the order of 1.5 eV. The lowest-energy excitations exhibit binding energies on the order of a few hundred meV and the corresponding electron-hole pairs turn out to be weakly correlated interband transitions with essentially single-particle character. Our results [3] offer unprecedented insight into the intrinsic properties of Na_2KSb and NaK_2Sb and are expected to stimulate further research on multi-alkali antimonides.

References:

- [1] C. Cocchi, S. Mistry, M. Schmeißer, J. Kühn, T. Kamps, *Condens. Matter.* **31**, 014002 (2018).
- [2] C. Cocchi, S. Mistry, M. Schmeißer, R. Amador, J. Kühn, T. Kamps, *Sci. Rep.* **9**, 18279 (2019).
- [3] R. Amador and C. Cocchi, to be submitted, (2020).

**Personal Information:****Name:** Richard Schier**Project:** B16**Office number:** (030)2093 66366**e-mail:** schierri@physik.hu-berlin.de

Electronic and optical properties of BCF-doped oligothiophenes from ab initio many-body theory

Richard Schier, Ana M. Valencia and Caterina Cocchi

Abstract:

Doping in organic semiconductors is an attractive research area for molecular electronics although the fundamental mechanisms ruling it are not yet fully understood. Recently, Lewis-acids such as tris(pentafluorophenyl)borane (BCF) [1,2] have been regarded with particular interest as a new class of dopants for organic semiconductors [3]. To gain insight into the microscopic properties of these materials, we investigate the electronic structure and optical properties of donor/acceptor interfaces formed by a single quarterthiophene (4T) molecule doped by a BCF species. For comparison, we consider also other adducts with 4T doped by hexafluorobenzene (C_6F_6) and the trihalide BF_3 . We carry out our study from first principles, in the framework of hybrid density-functional theory and many-body perturbation theory. For all systems, we find that the frontier orbitals are poorly hybridized and rather segregated on the donor or the acceptor depending on the specific level alignment of the system. As a consequence, the optical spectra of the systems appear almost as a superposition of those of the respective constituents. A quantitative analysis reveals interaction signatures in the form of dark excitations and peak shifts [4].

References:

- [1] Pingel *et al.*, Adv. Electron. Mater. **2**, 1600204 (2016).
- [1] Körte *et al.*, Angew. Chem. **56**, 8578 (2017).
- [3] Yurash *et al.*, Nat. Mater. **18**, 1327 (2019).
- [4] Schier *et al.*, to be submitted (2020)



Personal Information:

Name: J. Rika Simon

Project: A14

Office number: (030) 838-56052

e-mail: rika.simon@fu-berlin.de

Structural and electronic properties of F6-TCNNQ on monolayers of MoS₂ investigated by STM/AFM

J. Rika Simon, Christian Lotze and Katharina J. Franke

Abstract:

It has been shown previously that the charge transfer properties between an organic molecule and a monolayer of a transition metal dichalcogenide (TMDC) depend strongly on the nature of the substrate underneath the TMDC [1]. Here, we show preliminary work of combined scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) to investigate hexafluoro-tetracyano-naphthoquinodimethane (F6-TCNNQ) on MoS₂ on Au(111), as well as an outlook for possible future projects. F6-TCNNQ is of interest because of its high electron affinity and therefore an ideal candidate for investigating charge transfer. STM/AFM gives us access to the local adsorption structure of F6-TCNNQ while tunnelling spectroscopy can resolve the energy level alignment, which is indicative of charge transfer properties.

References:

- [1] S. Park, *et al.*, Comm Phys **2**, 109 (2019).



Personal Information:

Name: Ronaldo Rodrigues Pela
Project: B11
Office number: (030) 2093 66460
e-mail: ronaldo@physik-hu.berlin.de

All-electron real-time TDDFT implementation with Ehrenfest molecular dynamics

Ronaldo Rodrigues Pela and Claudia Draxl

Abstract:

Linearized augmented planewaves with local-orbitals (LAPW+lo) are arguably the most precise basis set to represent Kohn-Sham states. When employed within real-time time-dependent density functional theory (RT-TDDFT), they promise ultimate precision achievable for exploring the evolution of electronic excitations in time scales ranging from attoseconds to picoseconds. In this work, we present the implementation of RT-TDDFT in the full-potential LAPW+lo code **exciting** [1]. For relaxing the nuclear degrees of freedom, we include Ehrenfest molecular dynamics [2]. Our implementation provides the first step towards *ab initio* calculations of charge-carrier and exciton dynamics in HIOS.

References:

- [1] A. Gulans, *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
- [2] G. Kolesov, *et al.*, J. Chem. Theory Comp. **12**, 466 (2015).



Personal Information:

Name: Seon-Young Rhim

Project: B14

Office number: (030) 2093 7705

e-mail: seon-young.rhim@hu-berlin.de

Waveguide mode modulation with photochromic molecules for neuromorphic computing

Seon-Young Rhim, Giovanni Ligorio, Björn Kobin, Stefan Hecht and Emil List-Kratochvil

Abstract:

Artificial intelligence neural networks are already established in our everyday life and span from rail network planning to revealing chemical structures through data mining. The self-learning as the crucial property of an artificial neural network enables to recognize various patterns but also to create new patterns and solve new tasks with training sets without prewritten codes. Since these digitally realized artificial networks are inspired from the biological nervous system, the programmed networks consist of linked device units called perceptrons, which communicate using synaptic weights similar to the nervous cells. While these simulations are suitable for error analysis and network characterization, the operation could be more efficient in energy consumption by using analogous realized networks. Therefore, we demonstrate a full optically driven synaptic weight control by using polymeric waveguides. We exploit the total internal reflection effect to generate evanescent fields at the interfaces of the waveguide, which is highly sensitive to the dielectric function of the surrounding materials. By depositing photo-switchable molecules, we reversibly modulate the dielectric environment near the waveguide surfaces and thus the output spectrum by illuminating the switchable molecules with different wavelengths. Multi-state characteristics in the form of the output intensity can be shown for synaptic transduction for an employment in integrated photonic circuits.



Personal Information:

Name: Stefano Calati

Project: B9

Office number:

e-mail: calati@fhi-berlin.mpg.de

Dynamic Screening of Quasiparticles in WS₂ Monolayers

Stefano Calati, Samuel Palato and Julia Stähler

Abstract:

The low dimensional nature of transition metal dichalcogenides (TMDCs) and the resulting reduced screening significantly influence their non-equilibrium optical properties, as dynamic screening by photoexcited quasiparticles governs the transient response.

In this work, we investigate the role of different photoexcited quasiparticles on the dynamic response of WS₂ monolayers on SiO₂: excitons generated by resonant pumping and quasi-free carriers photoexcited by above-resonance pumping. Drastic changes in the reflectivity/Transmittance contrast upon photoexcitation are observed in both cases. The contribution of the exciton is isolated and modelled with a Lorentz oscillator. By using the Fresnel transfer matrix method we unravel the dynamics of the complex refractive index upon photoexcitation. Using a simple rate equation model, it is possible to reproduce the observed peak shift and broadening of the excitonic resonance and the extracted decay times from the multiexponential dynamics are reported. We compare then the dynamics of the exciton resonance upon resonant pumping for two different dielectric environment.

**Personal Information:****Name:** Victoria Taylor**Project:** B17**Office number:** +49 (0)30 8413-5134**e-mail:** taylor@fhi-berlin.mpg.de

Ultrafast spectroscopy and ultrafast electron diffraction studies of perovskites

Victoria Taylor, H el ene Seiler and Ralph Ernstorfer

Abstract:

Several studies have proposed that the high power conversion efficiencies of hybrid organic-inorganic halide perovskites are due to the organic cations orientating within the inorganic lattice to form stable (anti)ferroelectric domains at room temperature. [1-2] Two-dimensional infrared anisotropy measurements taken at the University of Bristol, were used to interrogate the reorientation of formamidinium cations (FA^+ , $\text{NH}_2\text{CHNH}_2^+$) in formamidinium lead iodide perovskite films. These measurements returned 470 ± 50 fs and 2.8 ± 0.5 ps time constants, meaning that any initial alignment of FA^+ molecules is short lived, precluding the presence of long-lived bulk (anti)ferroelectric domains. [3] Additional transient infrared measurements revealed a prominent vibrational transient feature arising from a vibrational Stark shift, indicating the formation of large polarons, which may explain the observed long charge-carrier lifetimes.

Ultrafast electron diffraction is an ideal technique for investigating dynamic lattice or phonon effects, such as polaron formation, since it directly probes lattice dynamics following photoexcitation. Nanocrystals of the inorganic perovskite CsPbBr_3 were investigated with this technique to monitor the lattice response following photoexcitation at the band-edge. The data indicates that electrons couple to acoustic phonons within 800 fs, as thermal expansion is observed on that timescale. Furthermore, additional structural dynamics beyond simple heating effects are also observed.

References:

- [1] M. C. G elvez-Rueda, *et al.*, J. Phys. Chem. C **120**, 16577 (2016).
- [2] J. M. Frost, *et al.*, Nano Lett. **14**, 2584 (2014).
- [3] V. C. A. Taylor, *et al.*, J. Phys. Chem. Lett. **9**, 895 (2018).

List of Names

Last Name	First Name	Session Name	Time	Project Number	Page Number
Akkoush	Alaa	Fundamental Inv. Methods	Wednesday 03:45 pm	A13	8
Amador	Raymond	Poster Session	Wednesday 01:00 pm	B16	34
Amsalem	Patrick	TMDCs	Thursday 01:20 pm	A8	16
Calati	Stefano	Poster Session	Wednesday 01:00 pm	B9	39
Christiansen	Dominik	Exciton Dynamics	Thursday 10:30 am	B12	11
Eljarrat	Alberto	Poster Session	Wednesday 01:00 pm	Z2	21
Gonzalez	Ignacio	Poster Session	Wednesday 01:00 pm	B11	25
Greben	Kyrylo	Fundamental Inv. Methods	Wednesday 03:15 pm	B15	6
Huynh	Dan-Nha	Plasmonics	Thursday 11:45 am	B10	14
Katzer	Manuel	Poster Session	Wednesday 01:00 pm	B12	27
Jacobs	Matheus	Poster Session	Wednesday 01:00 pm	B16	30
Kewes	Günter	Plasmonics	Thursday 11:30 am	B18	13
Klaue	Kristin	Poster Session	Wednesday 01:00 pm	A3	26
Krumland	Jannis	Exciton Dynamics	Thursday 10:00 am	B16	9
Liesfeld	Pauline	Poster Session	Wednesday 01:00 pm	A3	33
Lin	Hu	Poster Session	Wednesday 01:00 pm	A6	24
Lubeck	Sven	TMDCs	Thursday 01:35 pm	B11	17
Lungwitz	Dominique	Organic Semiconductors	Wednesday 11:30 am	A8	3
Maksimov	Dmitrii	Poster Session	Wednesday 01:00 pm	A13	22
Müller	Johannes	Fundamental Inv. Methods	Wednesday 03:00 pm	A12	5
Mutruc	Dragos	Poster Session	Wednesday 01:00 pm	A3	23
Neef	Alexander	Organic Semiconductors	Wednesday 11:15 am	B17	2
Palato	Samuel	Fundamental Inv. Methods	Wednesday 03:30 pm	B9	7
Pela	Ronaldo Rodrigues	Poster Session	Wednesday 01:00 pm	B11	37
Procida	Giovanni	Perovskites	Thursday 02:05 pm	B16	19
Raoufi	Meysam	Poster Session	Wednesday 01:00 pm	B7	31

Rhim	Seon-Young	Poster Session	Wednesday 01:00 pm	B14	38
Roczen	Maurizio	Family and career support during the COVID-19 pandemic	Thursday 12:00 pm	Z3	15
Rothe	Martin	Poster Session	Wednesday 01:00 pm	B2	29
Schier	Richard	Poster Session	Wednesday 01:00 pm	B16	35
Schloz	Marcel	Poster Session	Wednesday 01:00 pm	A12/Z2	28
Seiler	Hélène	Exciton Dynamics	Thursday 10:45 am	B17	12
Simon	Rika	Poster Session	Wednesday 01:00 pm	A14	36
Tanda Boncano	Boubacar	Organic Semiconductors	Wednesday 11:45 am	B9	4
Taylor	Victoria	Poster Session	Wednesday 01:00 pm	B17	40
Turkina	Olga	Exciton Dynamics	Thursday 10:15 am	B11	10
Vona	Cecilia	Perovskites	Thursday 01:50 pm	B11	18
Zhao	Yuhang	Poster Session	Wednesday 01:00 pm	B2	20
Zorn Morales	Nicolas	Poster Session	Wednesday 01:00 pm	B14	32

Contact

If you are experiencing technical problems, the organization team of the HYRW 2020 will gladly try to help you.

You can contact us via:

ZOOM: Write a private message to Seon-Young Rhim or Yuhang Zhao

E-mail: seon-young.rhim@physik.hu-berlin.de

yuhang.zhao@helmholtz-berlin.de

Impressum:

Editorial Team:

Alaa Akkoush, Dominique Lungwitz, Jie Ma,
Seon-Young Rhim, Yuhang Zhao, Maurizio Roczen.

Contact:

Sonderforschungsbereich 951
Zum Großen Windkanal 6
12489 Berlin

