

# Collaborative Research Centre 951



Hybrid Inorganic/Organic Systems for Opto-Electronics  
**Symposium 2020**

**10.09. – 11.09.2020**  
**Online Conference**  
Berlin, Germany

**Book of Abstracts**



Freie Universität  Berlin



**HZB** Helmholtz  
Zentrum Berlin



## Welcome

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## Welcome!

It is our pleasure to welcome you to the first international online symposium on Hybrid Inorganic/Organic Systems for Opto-Electronics (HIOS). Hosted by the Collaborative Research Centre (CRC) 951, the digital format of the HIOS Symposium will provide a new level for the open and creative scientific exchange of the latest achievements in the exciting field of hybrid inorganic/organic systems, comprising inorganic semiconductors, conjugated organic materials, and metal nanostructures.

During two days, sixteen invited talks, presented by international experts and by members of the CRC 951, will cover HIOS structure and morphology, electronic structure and control of inorganic/organic interfaces, charge and energy transfer, hybrid optical excitations, plasmonic phenomena, and much more. The scientific program is complemented by two poster sessions offering networking opportunities for all participants.

We are looking forward to see you soon on our screens and hope that you will enjoy your time at the  
**ONLINE HIOS SYMPOSIUM 2020.**

With best regards,

**Norbert Koch**  
Spokesperson CRC 951

**Oliver Benson**  
Vice-Spokesperson CRC 951



# Online Symposium on Hybrid Inorganic/Organic System for Opto-Electronics 2020

10.09 – 11.09.2020, Berlin, Germany

Time zone: CEST/UTC+2



September 10 <sup>th</sup> (Thursday)	
10.00	Welcome
10.10	<b>Xiaomin Xu</b> , Tsinghua University <i>From microstructure engineering of semiconductors to ultraflexible optoelectronics</i>
10.40	<b>Takhee Lee</b> , Seoul National University <i>Interface and surface control of transition-metal dichalcogenides with organic molecules and polymers</i>
11.10	<b>Emil List-Kratochvil</b> , HU Berlin <i>Active control over inorganic/organic material interface properties: Fundamental considerations and device applications</i>
11.40	Coffee Break
12.00	<b>Ute Kaiser</b> , Ulm University <i>Properties of low-dimensional materials by low-voltage TEM</i>
12.30	<b>Christoph Koch</b> , HU Berlin <i>Characterizing radiation sensitive hybrid inorganic/organic systems using elastic and inelastic electron scattering</i>
13.00	Lunch Break
14.00	Poster Session I
15.45	Coffee Break
16.00	<b>Mariana Rossi</b> , FHI Berlin <i>Structure and dynamics of inorganic/organic systems</i>
16.30	<b>Andreas Knorr</b> , TU Berlin <i>Ultrafast exciton-exciton interactions in (functionalized) atomically thin semiconductors</i>
17.00	Coffee Break
17.15	<b>Teri W. Odom</b> , Northwestern U <i>Quantum dot plasmon nanolasers</i>
17.45	<b>Eli Rotenberg</b> , Berkeley Lab <i>Nanoscale imaging of electronic states of 2D materials</i>

September 11 <sup>th</sup> (Friday)	
09.00	Poster Session II
10.45	Coffee Break
11.00	<b>Wei Chen</b> , NUS <i>Surface charge transfer doping enabled ohmic contacts for 2D materials</i>
11.30	<b>Gregor Witte</b> , PU Marburg <i>Hybrid-systems of organic and 2D materials: Interface structure and film formation</i>
12.00	<b>C.N.R. Rao</b> , JNCASR Bangalore <i>Linking nano-sheets of 2D materials to generate materials with new and novel properties</i>
12.30	Lunch Break
14.00	<b>Aleksandra Radenovic</b> , EPFL <i>Nanoscopy of 2D materials</i>
14.30	<b>Ralph Ernstorfer</b> , FHI Berlin <i>Ultrafast interfacial charge, exciton and phonon dynamics in van der Waals heterostructures</i>
15.00	Coffee Break
15.15	<b>Cecilia Mattevi</b> , IC London <i>Precise synthesis of 2D crystals for energy applications</i>
15.45	<b>Katharina Franke</b> , FU Berlin <i>Defects and molecular adsorbates on monolayers of MoS<sub>2</sub> on Au(111)</i>
16.15	Closing

Partners:



Poster Session I		
10.09.2020 (Thu.), 14.00 – 15.45 (CEST/UTC+2)		
Nr.	Presenter	Title
1	Alberto Eljarrat	Dispersion and temporal coherence of SPR modes in nanowires
2	Chengxu Shen	Morphology-controlled MoS <sub>2</sub> by low-temperature atomic layer deposition <i>will be presented in Poster Session II (September 11th)</i>
3	Christos Gatsios	Experimental investigation of thin epitaxial MoTe <sub>2</sub>
4	Dan-Nha Huynh	Different approaches to the hydrodynamic material model within the discontinuous Galerkin time-domain method
5	Holger-Dietrich Saßnick	Structural properties of a water monolayer on defective (110) rutile TiO <sub>2</sub> : a theoretical study
6	Hu Lin	Reversible switching of interfacial charge transfer with intercalating molecular layers
7	Ignacio Gonzalez Oliva	Electron-phonon coupling in hybrid inorganic/organic systems: a novel approach from first principles
8	Jannis Krumland	Ab initio modelling the ultrafast dynamics of laser-excited hybrid inorganic/organic interfaces in their environment
9	Jie Ma	Substrate dependent energy level alignment at a hybrid TMDC monolayer/molecular semiconductor interface
10	Johannes Müller	Enabling imaging and spectroscopy of electron beam sensitive hybrid materials
11	Juliane Mörsel	Impact of a metallic substrate on the opto-electronic properties of monolayer MoS <sub>2</sub>
12	Matheus Jacobs	Ultrafast charge transfer and vibronic coupling in the laser-excited F4TCNQ:H-Si(111) interface
13	Nicolas Zorn Morales	Switching impact of photochromic diarylethenes as self-assembled monolayer in organic light emitting diodes
14	Niklas Mutz	Excited state charge transfer at the phthalocyanine/MoS <sub>2</sub> Interface
15	Niko Nikolay	Fundamental properties of single-photon sources in hexagonal boron nitride
16	Oleksandra Shargaieva	Optical properties of iodoplumbate chains formed in solutions: from experiment to theory
17	Qiang Wang	Evolution of pure hydrocarbon hosts for the application in universal OLEDs
18	Robin Aydinonat	Optoelectronic properties of monolayer MoS <sub>2</sub> with sulfur vacancies
19	Ronaldo Rodrigues Pela	All-electron real-time TDDFT implementation with Ehrenfest molecular dynamics
20	Seon-Young Rhim	Waveguide mode modulation with photochromic molecules for neuromorphic computing
21	Stefan Kirstein	Individual tubular J-aggregates stabilized and stiffened by silica encapsulation
22	Thomas Kiel	Computational characterization of defect-state lasing in hybrid plasmonic-organic micro-cavities
23	Tobias Junghöfer	Challenges in evaporation of organic diradicals

Poster Session II		
11.09.2020 (Fri.), 09.00 – 10.45 (CEST/UTC+2)		
Nr.	Presenter	Title
24	Alaa Akkoush	Benchmarking electric field responses in all-electron electronic structure calculations
25	Alexander Neef	Viewing singlet fission in momentum space
26	Ana M. Valencia	Electronic properties of hybrid monolayer TMDC-conjugated molecule interfaces from first principles
27	Atindra Nath Pal	Nonmagnetic single-molecule spin-filter based on quantum interference
28	Biswajit Pabi	Post rupture evolution and jump to molecular contact in single molecular junction
29	Boubacar Tanda Bonkano	Excited state dynamics of unsubstituted terylene, a textbook molecule
30	Dominik Christiansen	Theory of short wavelength spectroscopy of two-dimensional HIOS: Exciton dynamics in tr-ARPES and X-ray response
31	Dragos Mutruc	Modulating guest uptake in core-shell MOFs with visible light
32	Hélène Seiler	Structural dynamics of pentacene single crystals and MoS <sub>2</sub> /pentacene heterostructures
33	Honghe Ding	In situ investigation of the Cu/CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub> interface in perovskite device
34	J. Rika Simon	Structural and electronic properties of F6-TCNNQ on monolayers of MoS <sub>2</sub> investigated by STM/AFM
35	Kristin Klaue	Donor–acceptor dihydropyrenes switchable with near-infrared light
36	Manuel Katzer	Anticrossing effects in photoluminescence excitation spectroscopy of quantum dots
37	Martin Rothe	Local chiral sensors for HIOS from self-assembled plasmonic nano-antenna-waveguide structures
38	Meysam Raoufi	Probing the charge carrier dynamics in hybrid layer stacks comprising a TMDC monolayer and an organic semiconductor
39	Michele Guerrini	Photoinduced electron dynamics of N-doped graphene quantum dots
40	Raymond Amador	Electronic and optical properties of Na <sub>2</sub> KSb and NaK <sub>2</sub> Sb from <i>ab initio</i> many-body theory
41	Richard Schier	Electronic structure of BCF-doped oligothiophenes from <i>Ab initio</i> many-body theory
42	Rongbin Wang	Direct observation of conductive polymer induced inversion layer in n-Si and correlation to solar cell performance
43	Sebastian Franke	Non-linear cavity QED effects in dissipative resonators using coupled quasinormal modes
44	Shubhrasish Mukherjee	Very high photoresponse from a few layered MoS <sub>2</sub> transistor
45	Stefano Calati	Dynamic screening of quasiparticles in WS <sub>2</sub> monolayers
46	Sviatoslav Kovalchuk	In-situ evaporation of molecular dopants on monolayer/bilayer TMDCs

## Important information at a glance

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### Important information at a glance

#### Time zones:

Please note, that all times in this booklet are given in **Central European Standard Time (CEST/UTC+2)** and the 24-hour clock format. For your convenience, we have listed the starting time of the first talk as well as the begin of the poster session for the most common time zones among the participants for both days of the symposium.

Countries (Time zone)	September 10 <sup>th</sup> (Thu.)		September 11 <sup>th</sup> (Fr.)	
	First Talk	Posters	First Talk	Posters
California (USA) (UTC-7)	01.00	05.00	02.00	00.00
Illinois (USA) (UTC-5)	03.00	07.00	04.00	02.00
United Kingdom (UTC+1)	09.00	13.00	10.00	08.00
Germany, France (UTC+2)	10.00	14.00	11.00	09.00
India (UTC+5.5)	13.30	17.30	14.30	12.30
Singapore, China (UTC+8)	16.00	20.00	17.00	15.00
Korea (UTC+9)	17.00	21.00	18.00	16.00

#### Recording of sessions:

The oral presentations, as well as the discussions will be recorded and made available solely to registered participants. You will receive a notification by ZOOM once the recording is in progress, which you have to confirm in order to stay in the ZOOM room. The poster sessions will NOT be recorded.



### **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 Maurizio Roczen or Christian Pugatschow 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 Thursday, 10<sup>th</sup> September 2020, starts at 10.00.

The first oral presentation on Friday, 11<sup>th</sup> September 2020, starts at 11.00.

## General Information

The presentations will be recorded and made available solely to registered participants of the symposium in a secured and password protected repository.

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 (see [ZOOM basics](#)). 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.

To encourage a lively discussion, questions which are asked in person are preferred over chatroom questions. However, all questions in the chatroom left unanswered will be collected and sent to the speaker directly. The answers to those questions will be made available on the secured repository of the HIOS Symposium 2020 homepage.

## From Microstructure Engineering of Semiconductors to Ultraflexible Optoelectronics

Xiaomin Xu

Shenzhen Geim Graphene Center, Tsinghua-Berkeley Shenzhen Institute (TBSI), Tsinghua University, Shenzhen (China)

Optical and electrical properties of organic and inorganic semiconducting materials are strongly determined by their microstructure. Consequently, the control and visualization of spatial structural variations are of paramount importance for applications in (opto)electronics. The realization of advanced optoelectronic functions, especially with a flexible device configuration, will ultimately benefit the Internet of Things (IoT) applications, which then requires an optimal combination of materials and devices at both microscopic and macroscopic levels.

Based on acene derivative molecules, we will address fundamentals in mastering the assembly of molecules and discuss distinct charge transport regimes in relation to the different microstructure of organic thin films [1]. We will then highlight the combined lateral force microscopy (LFM) and transverse shear microscopy (TSM) techniques that allow microstructure visualization of synthesized two-dimensional materials, identifying grain boundaries, crystal orientation, and strain fields unambiguously in a high-throughput and nondestructive manner [2]. One-step closer to the application, we will demonstrate a design of ultraflexible optoelectronics featuring extreme mechanical compliance, high performance, and operational stability, allowed by the combined strategies of microstructure and device engineering [3].

[1] X. Xu, Y. Yao, B. Shan, X. Gu, D. Liu, J. Liu, J. Xu, N. Zhao, W. Hu, Q. Miao, *Adv. Mater.* 28, 5276 (2016).

[2] X. Xu, T. Schultz, Z. Qin, N. Severin, B. Haas, S. Shen, J. N. Kirchhof, A. Opitz, C. T. Koch, K. Bolotin, J. P. Rabe, G. Eda, N. Koch, *Adv. Mater.* 30, 1803748 (2018).

[3] X. Xu, K. Fukuda, A. Karki, S. Park, H. Kimura, H. Jinno, N. Watanabe, S. Yamamoto, S. Shimomura, D. Kitazawa, T. Yokota, S. Umezumi, T.-Q. Nguyen, T. Someya, *Proc. Natl. Acad. Sci. U.S.A.* 115, 4589 (2018).

### **Interface and surface control of transition-metal dichalcogenides with organic molecules and polymers**

**Takhee Lee**

Department of Physics and Astronomy, Seoul National University, Seoul (Korea)

Transition metal dichalcogenide (TMD) two-dimensional (2D) atomic layered materials have recently drawn considerable attention as promising semiconductors for future ultrathin layered nanoelectronic device applications. Unlike graphene, TMD materials have a semiconductor band gap, for example, molybdenum disulfide ( $\text{MoS}_2$ ) that has been widely studied is known to have a direct band gap of  $\sim 1.9$  eV as a single  $\text{MoS}_2$  layer and an indirect band gap of  $\sim 1.2$  eV as a bulk  $\text{MoS}_2$  crystal.

In this talk, I will review our group research works on  $\text{MoS}_2$ -based nanoelectronic devices. In particular, I explain the following topics on the electrical properties of  $\text{MoS}_2$  field effect transistors (FETs); interface control by high energetic proton beam irradiation [1] and surface treatment by molecules for sulfur vacancy passivation [2]. If time allowed, I will explain on our other works related to 2D nanoelectronics such as inkjet-printed device application, molecular doping of 2D materials, etc [3].

[1] T.-Y. Kim et al., ACS Nano 8, 2774 (2014); J. Shin et al., Nanoscale 11, 13961 (2019).

[2] K. Cho et al., ACS Nano 9, 8044 (2015); K. Cho et al., Adv. Mater. 30, 1705540 (2018).

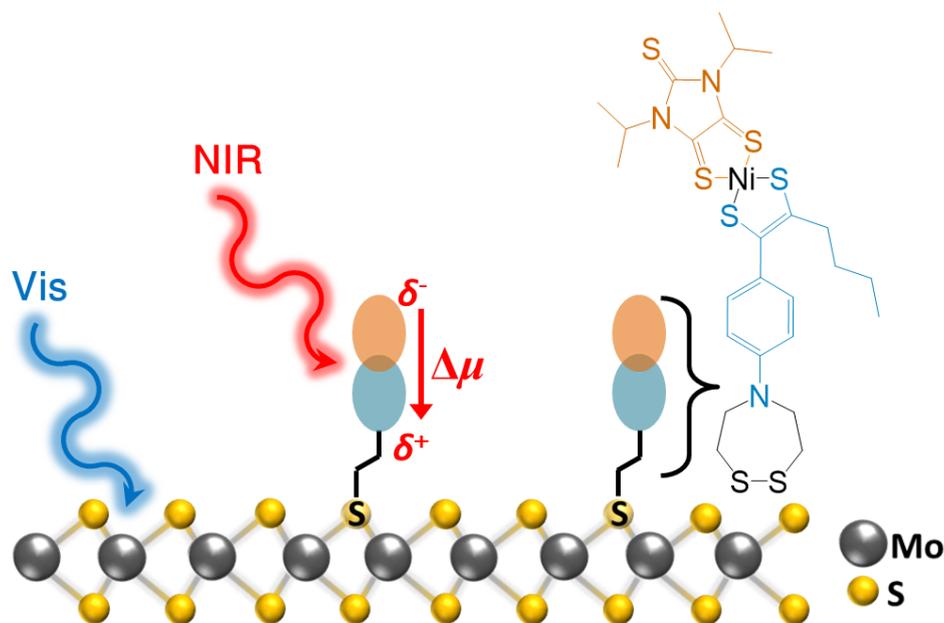
[3] T.-Y. Kim et al., ACS Nano 10, 2819 (2016); T.-Y. Kim et al., ACS Nano 11, 10273 (2017).

## Active control over inorganic/organic material interface properties: Fundamental considerations and device applications

Emil J. W. List-Kratochvil

Institut für Physik, Institut für Chemie & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin (Germany)  
Helmholtz-Zentrum für Materialien und Energie GmbH, HySPRINT Helmholtz Innovation Lab, Berlin (Germany)

The ability to form heterostructures from different materials, yet from the same material class, has revolutionized electronic and optical technologies during the past decades. To explore novel electronic and optoelectronic functionalities based on heterostructures in a natural next step we have turned to systematically explore hybrid inorganic/organic materials systems (HIOS) in heterostructures combining materials from dissimilar material classes. Among different aspects in this HIOS research endeavour, it was found that an in-depth understanding and control over the energy level alignment in HIOS is the key to attain novel electronic and optoelectronic functionalities. In particular, it has been found that self-assembled monolayers (SAMs) as interlayer between the inorganic and organic semiconductors provide many opportunities to control the work function and to modify injection as well as charge and energy transfer processes. Moreover, using more complex multifunctional SAMs based on optically switchable molecules such as dihydropyrenes, diarylethenes and solvatochromic molecules, allows going from static modifications of the HIOS interface towards in situ and operando tuning of the energy level alignment. In this contribution, we report on fundamental aspects of the SAM formation on different metal oxide and 2D semiconductors such as transition metal dichalcogenides, observations of switching processes and successful implementations in diode, light emitting diode, field effect transistor and neuromorphic plasmonic device structures.



Concept of near-infrared sensitization of MoS<sub>2</sub> by a solvatochromic dye

### **Properties of low-dimensional materials by low-voltage TEM**

**Ute Kaiser**

Central Facility of Electron Microscopy, Materials Science Electron Microscopy, Ulm University, Ulm (Germany)

It is a growing demand in materials sciences to unravel the atomic and electronic structure of low-dimensional materials to understand their atomic-defects-induced properties. For this purpose, a new type of transmission electron microscopes, the so-called SALVE instrument has been developed operating at electron accelerating voltages between 80kV and 20kV. It allows undercutting most of the materials knockon damage thresholds and enables sub-Ångstroem resolution down to 40kV by correcting not only the geometrical aberrations of the objective lens but also its chromatic aberration, to study dynamic of interactions. Using the SALVE instrument, we report on properties of pristine and electron-beam functionalised two-dimensional materials including various transition metal dichalchogenides (TMDs) and Lifunctionalised bi-layer graphene. In addition we report on completely new insights into nucleation of metals and into metal bonding. The latter two examples we study inside an electron-transparent test tube.

## Characterizing radiation sensitive hybrid inorganic-organic systems using elastic and inelastic electron scattering

**Christoph Koch**<sup>1</sup>, Johannes Müller<sup>1</sup>, Alberto Eljarrat<sup>1</sup>, Benedikt Haas<sup>1</sup>, Zdravko Kochovski<sup>1,2</sup>, Ondrej Krivanek<sup>3,1</sup>

<sup>1</sup> Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin (Germany)

<sup>2</sup> Helmholtz-Zentrum Berlin (HZB), Berlin (Germany)

<sup>3</sup> Nion Company, Kirkland, WA (USA)

Hybrid inorganic-organic systems (HIOS) may have unique (optoelectronic) properties due to the atomic and electronic structure at the interface between its organic and inorganic components. Characterizing such systems requires probes that are sensitive not only to the outer surface, but also to the internal interfaces between its constituents. Intentional or unintentional heterogeneity of such systems at the nanoscale often requires that such methods are also capable of providing measurements localized on the nanoscale. Fast electrons in the transmission electron microscope (TEM) fulfill all these requirements and may interact elastically (kinetic energy of the electron is the same before and after the scattering process) or inelastically (the electron transfers energy to the sample or gains energy from it) with the material being probed and may be focused to a probe less than one Ångström in diameter. While the elastic interaction probes the local electrostatic potential projected along the electron beam trajectory, the inelastic interaction provides information about electronic and vibrational excitations in the material. In this talk I will present different strategies (minimizing dose, reducing beam energy, probing excitations without sending the beam through the material, characterizing shock-frozen materials, etc.) of how we avoid damage when characterizing the atomic structure, strain, crystallographic orientation, optical dispersion and other properties of HIOS in the TEM and present results obtained from different systems we have characterized as part of our collaborations with various partners from the CRC 951 (organic thin films on TMDC, coated Ag nanowires, one or few layer thin TMDC films, etc.).

### Structure and Dynamics of Inorganic/Organic Systems

Mariana Rossi

Theory Department, Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin (Germany)  
Max Planck Institute for the Structure and Dynamics of Matter, Hamburg (Germany)

In weakly bonded systems, the nuclear fluctuations induced by temperature can completely change the structure, the thermodynamic equilibrium, and also the electronic structure of materials. In addition, given the ubiquitous presence of light nuclei in organic materials, not only the electrons but also the nuclear fluctuations must be treated within the first principles of quantum mechanics.

In this talk, I will show how we achieve an all-atom, all-electron quantum description of these systems by developing methodology and tools that allow joining density-functional theory calculations to path integral methods. I will show situations, involving organic/inorganic interfaces, where we have solved questions related to level broadening in semiconductor interfaces, pronounced temperature dependence of electronic properties and charge transfer at interfaces, as well as apparently contradictory observations in hydrogen transfer reactions. None of this would be possible if the atomic structure of the systems was unknown or incorrect. This is why we also conduct exhaustive ab initio structure searches of single molecules and self-assembled monolayers and develop ab initio random structure search program packages, optimising force evaluations and geometry relaxations of weakly bonded interfaces.

## Ultrafast exciton-exciton interactions in (functionalized) atomically thin semiconductors

Dominik Christiansen, Florian Katsch, Robert Salzwedel, **Andreas Knorr**, Malte Selig  
 Nichtlineare Optik und Quantenelektronik von Halbleitern, Institut für Theoretische Physik,  
 Technische Universität Berlin, Berlin (Germany)

Atomically thin semiconductors constitute a remarkable playground for exciton physics in two dimensions. This involves optically accessible (bright) as well as spin- and momentum-forbidden (dark) excitonic states including intravalley and intervalley excitations [1, 2]. The nonlinear, coherent exciton dynamics induced by short light pulses results from the interplay of intrinsic exciton-exciton [3, 4] and exciton-phonon [5] interactions. Here, we present applications of the theory to:

- exciton-phonon and exciton-exciton scattering induced coherence decay [5, 6, Fig.1a],
- detection of exciton wave functions in time resolved ARPES [7, Fig.1b], and
- atomically thin semiconductors functionalized with metal-nanoparticles or organic molecules, induced by different charge-, Dexter- or Förster-type transfer processes.

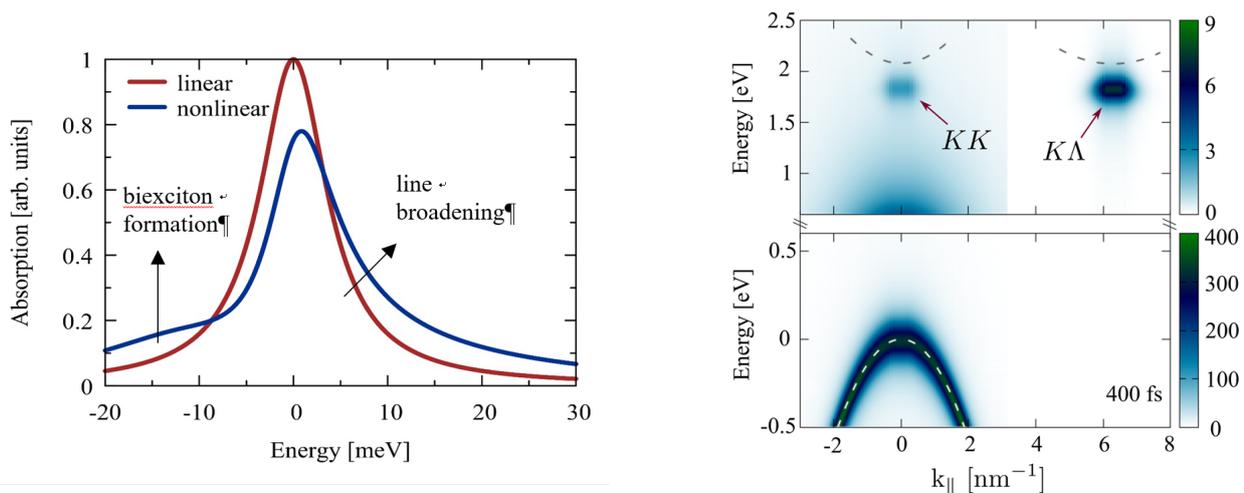


Fig. 1: (a) Linear and nonlinear absorption of monolayer  $\text{WSe}_2$  at 10 K for excitation with linearly polarized light. The nonlinear absorption shows a line broadening and the formation of a biexciton resonance. (b) Photoemission signal of monolayer  $\text{WSe}_2$  at 77 K for a time delay of 400 fs. The relaxation of electrons into the  $\Lambda$  valley results in momentum-forbidden  $K\Lambda$  excitons shown as an excitonic peak below the  $\Lambda$  conduction band (dashed) at  $k_{\parallel} \approx 6 \text{ nm}^{-1}$ . The weaker signal at the K point is due to  $KK$  excitons and momentum-forbidden  $KK'$  excitons.

- [1] G. Wang et al., Rev. Mod. Phys. 90, 021001 (2018).  
 [2] E. Malic et al., Phys. Rev. Materials 2, 014002 (2018).  
 [3] V. M. Axt and T. Kuhn, Rep. Prog. Phys. 67, 433 (2004).  
 [4] F. Katsch, et al., Phys. Stat. Sol. (b) 255, 1800185 (2018) and 2D Mater. 7, 015021 (2020).  
 [5] M. Selig, et al., Phys. Rev. Research. 1, 022007 (2019).  
 [6] F. Katsch et al., Phys. Rev. Lett. 124, 257402 (2020).  
 [7] D. Christiansen et al., Phys. Rev. B 100, 205401 (2019).

### **Quantum Dot Plasmon Nanolasers**

**Teri W. Odom**

Department of Chemistry, Northwestern University, Evanston, IL (USA)

Miniaturized light sources are critical for integrated, on-chip photonic devices. This talk will describe a nanolaser design based on colloidal CdSe-CdS core-shell quantum dots (QDs) conformally coated on two-dimensional arrays of plasmonic nanoparticles. These QD-plasmon lasers can show directional emission by exploiting high symmetry points in the lattices and tailorable polarization patterns depending on the QD film thickness. We will discuss prospects for achieving any desired lasing emission angle from this room-temperature hybrid nanolaser.

## Nanoscale Imaging of Electronic states of 2D Materials

**Eli Rotenberg**

Lawrence Berkeley National Laboratory, Berkeley, CA (USA)

Angle-resolved photoemission spectroscopy (ARPES) was developed for the determination of the electronic bandstructure of solids. In the last 10 years or so, ARPES energy/momentum resolution has improved to the point where it can illuminate more subtle electronic aspects, such as symmetry breaking and the many-body interactions (MBIs) that determine electronic and optical behavior. These MBIs involve exchange of momentum among electrons or with excitations such as phonons, and can therefore couple to nanoscale structures. By controlling the structure of materials on the nanoscale, we can therefore hope to control or enhance the ground state properties of materials through nanoscale engineering. With decreasing probe sizes, we could also open up new studies of materials in device form, with applied fields and currents.

This dream has motivated the development of ARPES with nanoscale spatial resolution (nanoARPES), in order to probe these effects. I will give an overview of the development of this technique at the Advanced Light Source in Berkeley, and give some examples of recent research.

### Surface Charge Transfer Doping Enabled Ohmic Contacts for 2D Materials

Wei Chen

Department of Physics, National University of Singapore (Singapore)  
Department of Chemistry, National University of Singapore (Singapore)  
Joint School of National University of Singapore and Tianjin University,  
International Campus of Tianjin University, Fuzhou (China)

Two-dimensional (2D) layered materials like graphene and transition metal dichalcogenides (TMDs) have been considered as promising building blocks for the next generation nanoelectronic devices, showing great potentials to extend the scaling limits existing in silicon based complementary metal-oxide-semiconductor field-effect-transistors (CMOS-FET) as well as to serve as a high mobility alternative to organic semiconductors for flexible electronic and optoelectronic devices. However, the existence of large contact resistance at the interface between the TMDs semiconductor and any bulk (or 3D) metal drastically restrains the intrinsic transport properties of materials and the performance of realistic devices. Thus, it is a crucial to optimize the contacts and lower the contact resistance between 2D semiconductors and metal electrodes.

In this talk, I will summarize and discuss our recent work for the development of scalable Ohmic contact engineering approaches to 2D materials that can be easily integrated into existing semiconductor device production processes. We will focus on the Ohmic contact to 2D materials enabled by surface charge transfer doping induced semiconductor-to-metal phase transition, and the demonstration of high performance 2D materials based electronic devices with Ohmic contact.

## Hybrid-Systems of Organic and 2D Materials: Interface Structure and Film formation

Gregor Witte

Department of Physics, Philipps-Universität Marburg, Marburg (Germany)

Van der Waals (vdW) bound layered compounds have attracted large scientific attention because these 2D-materials can be processed as ultrathin or even single layers revealing outstanding electronic properties. As their electronic properties can be very different ranging from semimetals to semiconductors and insulators, stacking them creates interesting perspectives for future technological applications. In addition to this strategy, the combination of such 2D materials with organic semiconductors (OSC) has recently been discussed as a promising extension [1]. Such OSC-2D material hybrid systems have the advances that opto-electronic properties of the OSCs are easily tunable through chemical synthesis, while the 2D layers provide very sharp internal interfaces where notable chemical interactions or even chemical interface reactions can be excluded, so that the molecular materials maintain their intrinsic electronic properties even at the interface. On the other hand, as the optoelectronic properties of OSC materials depend sensitively on the molecular orientation and packing motifs, it is of key importance to control the microstructure of such hybrid systems - especially at the interface [2].

Here, I will discuss some examples of interface structures and the subsequent film formation of prototypical OSC materials on various 2D materials including graphite, transition metal dichalcogenides (TDMCs) and hexagonal boron nitride (hBN). Due to the generally weak molecule-substrate interactions, the resulting film structures depend critically on the crystalline surface quality and are largely affected or even controlled by defects such as steps. To determine the intrinsic interface structure, OSC films were also grown on single crystalline substrates which represent the most ideal surfaces, while sometimes very different film structures are found on exfoliated flakes. Acenes form highly ordered crystalline films which exhibit a point-on-line epitaxy on the various 2D materials, of which structure can be elegantly determined by means of optical anisotropy measurements even on small samples. Interestingly, acenes such as pentacene (PEN) and perfluoro-pentacene (PFP) experience a somewhat larger molecule-substrate interaction on  $\text{MoS}_2$  than on insulators like  $\text{SiO}_2$ , which allows to prepare nominal monolayer films by selective desorption of excess multilayers as frequently done on metals. However, these "monolayers" do not condensate and instead form a quasi-2D liquid, while condensation takes place only upon multilayer formation. This effect is explained by repulsive mutual interaction between the planar adsorbed acenes as found before also on Ag(111) surfaces [3]. While this phenomenon occurs for unitary films of both PEN and PFP, a co-deposition leads to a mutual stabilization of the molecular entities even in sub-monolayer films. Such an electrostatic stabilization is also achieved when using acenes of which rim is unilaterally fluorinated, thereby introducing a self-stabilization as demonstrated for the newly synthesized unilaterally fluorinated F6PEN [4].

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[2] T. Breuer et al., Phys. Status Solidi RRL 10, 905 (2016).

[3] M. Marks et al., J. Phys. Chem. C. 116, 1904 (2012).

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**Linking nano-sheets of 2D materials to generate materials  
with new and novel properties**

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## Nanoscopy of 2D materials

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The simplicity and versatility of optical microscopy make it from the start the workhorse technique in the characterization of 2D materials [1]. Optical microscopy is used to locate and determine the thickness of the 2D material by measuring its optical contrast with respect to the Si/SiO<sub>2</sub> substrate [2]. Although in terms of technology, the large-area growth of 2D materials is about to be mastered soon, as-grown 2D materials still host abundant and different types of defects such as vacancies, adatoms, grain boundaries (GBs), edges, and impurities, which strongly influence their properties [3]. In most cases, the presence of defects is disadvantageous. However, not all defects in 2D materials are detrimental. Some 2D materials have been shown to host defects that can serve as single-photon emitters (SPEs) at cryogenic temperatures for TMDs [4-7] and room temperature for h-BN [8]. This discovery has motivated the search for single-photon sources in other 2D materials and efforts that aim to engineer the defects in well-controlled locations either using strain-induced potential traps [9] or via quantum dot confinement [7]. We have explored the single molecule localization microscopy to characterize defects in hexagonal boron nitride [10]. In addition to precise location of the optically active defects we record as well their spectral properties using spectral SMLM [11] and we use them as a platform that allowed us to track excess protons in interfacial water [12].

Focusing on sulfur-vacancies in TMDs, we demonstrate large-scale mapping of non-emissive defects by coupling single-molecule localization microscopy with fluorescent labelling using thiol chemistry, reminiscent of Point Accumulation for Imaging in Nanoscale Topography (PAINT). We found non-homogenous resonance energy transfer efficiency on MoS<sub>2</sub> dependent on the defect structure (grain boundaries and line defects). Moreover, our method allows us to probe the defects that are chemically active in aqueous conditions and reveal insights of the interaction between the thiol group and the sulfur-vacancy. Importantly, our methodology paves the way for in-situ and spatially-resolved monitoring of the interaction between the chemical agent and the defects in 2D materials that has general implications for defect engineering in aqueous condition. With the versatile chemical labelling strategy, our method is generally applicable to a variety of defects in 2D materials [13].

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[13] M. Zhang et al., arXiv:2006.12181 (2020).

### Ultrafast interfacial charge, exciton and phonon dynamics in van der Waals heterostructures

Shuo Dong, Tommaso Pincelli, Thomas Vasileiadis, Helene Seiler, Samuel Beaulieu, Alexander Neef, Daniela Zahn, Maciej Dendzik, Julian Maklar, Yoav W. Windsor, Sang Lee, Patrick Xian, Martin Wolf, Laurenz Rettig, **Ralph Ernstorfer**  
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We investigate real-time dynamics of photo-induced carrier, energy, and phonon dynamics in the prototypical van der Waals heterostructure  $WSe_2$ -graphene and Au-decorated  $WSe_2$  with pump-probe techniques providing momentum-space information. The dynamics of electrons and excitons is observed with four-dimensional time- and angle-resolved photoelectron spectroscopy (trARPES), featuring a high-repetition rate XUV laser source and momentum microscope detector. Depending on the nature of the photo-excited state in the  $WSe_2$ -graphene heterostructures, we observe carrier scattering between the K valleys of graphene and the K and  $\Sigma$  valleys of the  $WSe_2$  conduction band, or exciton transfer from the semiconductor to the semimetal. In case of  $WSe_2$  decorated with epitaxial nano-islands of Au, we observe signatures of plasmonically enhanced two-photon absorption in the transition metal dichalcogenide and subsequent ultrafast electron transfer. Femtosecond electron diffraction additionally reveals the dynamics of vibrational energy transfer across the interface. We will discuss the extension of this approach to inorganic-organic systems.

## Precise synthesis of 2D crystals for energy applications

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Layered transition metal dichalcogenides (TMDs) display a variety of structural polymorphs defined by the symmetry of transition metal coordination polyhedra. Tailoring the lattice symmetry within individual TMD layers enables to achieve very different electronic properties ranging from semiconducting (2H phase) to metallic and semimetallic (1T/1T' phases) with the same material composition. Exhibiting metallic behaviour, the metastable 1T' phases are particularly appealing for electrocatalytic hydrogen production from acid water as they approach Pt performance. The direct synthesis of the metastable phases of high purity and in measurable quantities remains challenging. Here, we present our work on the bottom-up synthesis of the metastable 1T' phase of WSe<sub>2</sub> based on the reaction between molecular precursors in liquid phase [1]. We design a kinetically-controlled bottom-up synthesis from molecular precursors to enable the formation of the metastable phase. We further demonstrate that the 1T' phase is stable up to 400°C and it is convertible into the semiconducting 2H phase at higher temperatures, making it suitable for a wide range of applications. The 1T' WSe<sub>2</sub> nanosheets exhibit a metallic nature evidenced by an enhanced electrocatalytic activity for hydrogen evolution reaction as compared to the 2H WSe<sub>2</sub> and different sulphides. Further, we demonstrate how this synthesis approach can be applied to design of new catalytic systems.

[1] M. S. Sokolikova, P. C. Sherrell, P. Palczynski, V. L. Bemmer, C. Mattevi, *Nat. Commun.* 10, 712 (2019).

### Defects and molecular adsorbates on monolayers of MoS<sub>2</sub> on Au(111)

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Monolayers of transition metal dichalcogenides (TMDCs) have matured to an important class of two-dimensional materials. Many of them are semiconductors, which are important for optoelectronic devices. Here, we grow monolayers of MoS<sub>2</sub> on a Au(111) surface, following the preparation methods from earlier publications (see, e.g. [1]). Using a combination of scanning tunneling microscopy and atomic force microscopy, we identify a variety of point defects. These are missing sulfur atoms as well as interstitial sites inside the MoS<sub>2</sub> layer. Tunneling spectra on these defects reveal characteristic states, which have already been predicted by DFT calculations in similar systems [2, 3].

Furthermore, we explore the monolayers of MoS<sub>2</sub> on Au(111) as a substrate for organic molecules. We find that adsorbed molecules exhibit a large set of vibronic states [4, 5, 6]. The line shape of these resonances suggests a prolonged lifetime of the electronic excitations as well as a small electron-phonon coupling in the MoS<sub>2</sub> layer.

- [1] S. G. Sorensen et al., ACS Nano 8, 6788 (2014).
- [2] J. D. Fuhr et al., Phys. Rev. Lett. 92, 026802 (2004).
- [3] C. González et al., Nanotechnology 27, 105702 (2016).
- [4] N. Krane et al., ACS Nano 12, 11698 (2018).
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- [6] G. Reecht et al., Phys. Rev. Lett. 124, 116804 (2020).



## Poster Session I

The first Poster Session starts on Thursday, 10<sup>th</sup> September 2020, at 14.00.

The second Poster Session starts on Friday, 11<sup>th</sup> September 2020, at 09.00.

### General Informaion

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. For technical reasons, only the host of the meeting (Maurizio Roczen) can assign you to a room. Please send your desired room number to the host via the chat function. You will then be assigned to the according poster. To visit another poster, please leave the room you are currently in and again send your desired room number to the host. To leave a breakout room, click 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.

**01 Dispersion and temporal coherence of SPR modes in nanowires**Alberto Eljarrat<sup>1</sup>, Martin Rothe<sup>1</sup>, Günter Kewes<sup>1</sup>, Oliver Benson<sup>1</sup>, Yuhang Zhao<sup>2</sup>, Yan Lu<sup>2</sup>, Christoph T. Koch<sup>1,3</sup><sup>1</sup>Institut für Physik, Humboldt-Universität zu Berlin, Berlin (Germany)<sup>2</sup>Institute for Electrochemical Energy Storage, Helmholtz-Zentrum Berlin, Berlin (Germany)<sup>3</sup>IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin (Germany)

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 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 MPDI dye molecules and silica-cover. Moreover, traces of the dye molecule are found in the spectra, hinting the possibility of direct detection of these molecules. The STEM-EELS technique proves especially 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  $\mu\text{m}$  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.

**02 Morphology-controlled MoS<sub>2</sub> by low-temperature atomic layer deposition**

This poster will be presented in Poster Session II on Friday, September 11th!

Chengxu Shen<sup>1</sup>, Muhammad Hamid Raza<sup>1</sup>, Patrick Amsalem<sup>2</sup>, Norbert Koch<sup>2</sup>, Nicola Pinna<sup>1</sup><sup>1</sup>Institut für Chemie and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin (Germany)<sup>2</sup>Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin (Germany)

Two-dimensional (2D) transition metal dichalcogenides (TMDs) such as MoS<sub>2</sub> are promising materials which have been applied in multifarious areas such as sensing, catalysis, and energy storage [1]. Due to their peculiar charge-transport properties, it is always desired to control their morphologies from horizontal basal-plane oriented smooth layers to vertical nanostructures [2]. Due to the high conformality, atomic layer deposition (ALD) exhibits promising potential in the precise control of the thicknesses and morphologies of the deposited layers, especially for the preparation of complex nanostructures [3].

In our research, we established a low-temperature thermal ALD process for MoS<sub>2</sub> deposition using Bis(t-butylimino)bis(dimethylamino) molybdenum(VI) and H<sub>2</sub>S as precursors. The morphologies of the deposited MoS<sub>2</sub> are tuned from smooth films to vertical nano-flakes by controlling reaction conditions. Noticeably, the deposited MoS<sub>2</sub> nanostructures show morphology-dependent optical properties.

[1] T. Jurca, M. J. Moody, A. Henning, J. D. Emery, B. Wang, J. M. Tan, T. L. Lohr, L. J. Lauhon, T. J. Marks, *Angew. Chem. Int. Ed. Engl.* 56, 4991 (2017).

[2] J. Hamalainen, M. Mattinen, K. Mizohata, K. Meinander, M. Vehkamäki, J. Raisanen, M. Ritala, M. Leskela, *Adv. Mater.* 30, e1703622 (2018).

[3] C. Marichy, M. Bechelany, N. Pinna, *Adv. Mater.* 2012, 24 (2017).

### 03 Experimental investigation of thin epitaxial MoTe<sub>2</sub>

Christos Gatsios<sup>1</sup>, Polychronis Tsipas<sup>2</sup>, Sotirios Fragkos<sup>2</sup>, Dimitra Tsoutsou<sup>2</sup>, Athanasios Dimoulas<sup>2</sup>, Yannis Raptis<sup>1</sup>

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Transition metal dichalcogenides is a promising class of materials showing remarkable properties for novel technological applications. Their layered structure with strong in-plane bonds and weak out-of-plane bonds enables the exfoliation into two-dimensional layers similar to graphene. MoTe<sub>2</sub> is an attractive candidate which exhibits a variety of electronic phases depending on its specific structural phase. Apart from the conventional semiconducting phase, MoTe<sub>2</sub> exhibits a semi-metallic phase which is accompanied by exciting topological properties that rise from the strong spin-orbit coupling [1]. Throughout this study, thin films of MoTe<sub>2</sub> were grown by molecular beam epitaxy (MBE) and were investigated in-situ by means of photoelectron spectroscopy and scanning tunneling microscopy. It was found that MoTe<sub>2</sub> exhibits semi-metallic behavior, thus could be a candidate for novel spintronic applications.

[1] J. A. Reyes-Retana, F. Cervantes-Sodi, Sci. Rep. 6, 24093 (2016).

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

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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.

[1] K. Busch, M. König, J. Niegemann, Laser Photonics Rev. 5, 773 (2011).

[2] D. Huynh et al., Appl. Phys. B 122, 1 (2016).

## 05 Structural properties of a water monolayer on defective (110) rutile TiO<sub>2</sub>: a theoretical study

Holger-Dietrich Saßnick<sup>1,2</sup>, Victor G. Ruiz<sup>1</sup>, Caterina Cocchi<sup>2,4</sup>, Joachim Dzubiella<sup>1,3</sup>, Sebastien Groh<sup>3</sup>

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Photocatalytic water splitting is a process for clean energy with promising technological applications to reduce environmental pollution and mitigate climate change. Rutile TiO<sub>2</sub> (110) has become the prototypical oxide surface in surface science and its interaction with water a model system for the water-oxide interface. However, modelling the interfacial system is still a challenging task due to various processes that take place on very different timescales. To overcome the limitations of different theoretical models and to gain an improved understanding of defect altered properties, a multiscale approach is used to establish the relation between the hydroxylation state and the surface diffusion of proton.

We investigate the impact of healed oxygen vacancy defects upon the degree of hydroxylation and the structural properties of the water monolayer under ambient conditions. Surface diffusion, analyzed using a one dimensional random walk model, is presented and discussed with regard to the hydroxylation state. The performed simulations include classical reactive molecular dynamics and electronic structure calculations based on density functional theory.

## 06 Reversible switching of interfacial charge transfer with intercalating molecular layers

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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.

[1] H. Lin, A. Schilo, A.R. Kamoka, N. Severin, I. M. Sokolov, J. P. Rabe, Phys. Rev. B 95, 195414 (2017).

## 07 Electron-phonon coupling in hybrid inorganic/organic systems: a novel approach from first principles

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The coupling between electrons and crystal-lattice vibrations (phonons) plays an important role in a wide range of physical phenomena such as the temperature dependence of the electrical resistivity, carrier mobility and the emergence of conventional superconductivity [1]. Only in the last decade the computational tools to study electron-phonon interactions (EPI) from first-principles have become accessible. Nevertheless, due to their high computational cost, EPI calculations are mostly restricted to systems with a few atoms per unit cell. We are developing a novel first-principles approach to extend EPI calculations to hybrid inorganic/organic systems (HIOS) based on the electronic and vibrational properties of the constituents. All calculations are performed using *exciting*, a full-potential all-electron code based on the linearized augmented plane-wave plus local orbitals (LAPW + lo) method [2]. We will present the formalism as well as preliminary results on the hybrid system consisting of a monolayer of pyridine on top of two dimensional monolayer MoS<sub>2</sub>.

[1] F. Giustino, Rev. Mod. Phys. 89, 015003 (2017).

[2] A. Gulans et al., J. Phys. Condens. Matter 26, 363202 (2014).

## 08 *Ab initio* modelling the ultrafast dynamics of laser-excited hybrid inorganic/organic interfaces in their environment

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We explore the light-induced dynamics in hybrid organic/inorganic complexes by means of real-time time-dependent density functional theory in conjunction with Ehrenfest molecular dynamics. This approach offers an *ab initio* and non-adiabatic description of the coupled electron-nuclear dynamics on the sub-picosecond time scale. In this way, it is possible to assess the role of vibronic coupling in the dynamics of ultrafast excitations and charge-transfer processes. The electron dynamics are described quantum-mechanically and analyzed in terms of orbital populations and the electron density, while the nuclear motion is treated classically and interpreted by considering time-dependent bond lengths and normal coordinates [1]. We explore these effects in hybrid systems and in their building blocks: Vibronic couplings are examined in organic (donor/acceptor) complexes, while *k*-resolved population dynamics are monitored in transition metal dichalcogenide (TMDC) monolayers. Moreover, we further develop the formalism of the polarizable continuum model to include interactions with the environment in the optical response of the systems. This framework [2] allows us to investigate the influence of screening substrates, solvents, and plasmonic nanoparticles on both the static and dynamic regime.

[1] J. Krumland, A. M. Valencia, S. Pittalis, C. A. Rozzi, C. Cocchi, J. Chem. Phys. in print (2020); arXiv:2003.08669

[2] J. Krumland, G. Gil, S. Corni, C. Cocchi, in preparation (2020).

## 09 Substrate dependent energy level alignment at a hybrid transition metal dichalcogenide monolayer/molecular semiconductor interface

Jie Ma<sup>1,2</sup>, Patrick Amsalem<sup>1</sup>, Xiaomin Xu<sup>1</sup>, Thorsten Schultz<sup>1,2</sup>, Dongguen Xin<sup>1</sup>, Norbert Koch<sup>1,2</sup>

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Combining transition metal dichalcogenides (TMDCs) and molecular semiconductors (MSCs) is an attractive route for forming van der Waals heterostructures [1] with novel (opto-)electronic properties. Such properties are expected to strongly depend on the energy level alignment at the corresponding interfaces, which may also be influenced by the employed supporting substrate [2]. In particular, a detailed microscopic understanding of the impact of the substrate electrical properties on the energy level alignment at TMDC/MSC interfaces is still lacking. Here, we determined by angle-resolved ultraviolet and X-ray photoelectron spectroscopy the electronic band line-up at a  $WS_2/C_{60}$  interface supported by either an insulating or a semi-metallic substrate. These insights can be useful for future design of functional heterostructures with tailored (opto-)electronic properties based on the combination of 2D and molecular semiconductor materials.

[1] D. Jariwala et al., Nano Lett. 16, 497 (2016).

[2] P. Soohyung et al., Commun. Phys. 2, 109 (2019).

## 10 Enabling imaging and spectroscopy of electron beam sensitive hybrid materials

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We modified our scanning electron microscope (SEM) to acquire diffraction patterns of thin samples in transmission at each scan position (4D-STEM [1]). 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, 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  $<5meV$  energy resolution [2].

[1] C. Ophus, Microscopy and Microanalysis 25, 563-582 (2019).

[2] O. L. Krivanek et al., Ultramicroscopy 203, 60-67 (2019).

## **11** Impact of a metallic substrate on the opto-electronic properties of monolayer MoS<sub>2</sub>

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Two-dimensional MoS<sub>2</sub> is a semiconductor with a direct band gap, reduced dielectric screening, strongly bound excitons, and intense charge-carrier interaction. These properties place MoS<sub>2</sub> among the most interesting candidates for the next-generation of opto-electronic devices. However, these properties are sensitive to the dielectric environment, and are different for isolated MoS<sub>2</sub> and MoS<sub>2</sub> deposited on a substrate. Therefore, it is important to understand the impact of a substrate on the band structure and on excitonic effects. In this work, we perform ab-initio calculations with the full-potential all-electron package `exciting` [1] to investigate the influence of a Au(111) substrate of different thickness on the opto-electronic properties of MoS<sub>2</sub>.

[1] A. Gulans et al., J. Phys.: Condens. Matter 26, 363202 (2014).

## **12** Ultrafast charge transfer and vibronic coupling in the laser-excited F4TCNQ:H-Si(111) interface

Matheus Jacobs<sup>1</sup>, Jannis Krumland<sup>1</sup>, Ana M. Valencia<sup>1</sup>, Haiyuan Wang<sup>2</sup>, Mariana Rossi<sup>2</sup>, Caterina Cocchi<sup>1</sup>

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Hybrid inorganic/organic systems (HIOS) are intriguing materials for opto-electronics, where interfacial charge transfer is primarily responsible for unique electronic structure and optical response. It is therefore essential to gain insight into this process also beyond the static picture. Ab initio methods based on real-time time-dependent density-functional theory coupled to Ehrenfest molecular dynamics are ideally suited for this problem [1]. Here, we investigate a laser-excited HIOS formed by the electron accepting molecule F4TCNQ physisorbed on a hydrogenated silicon cluster, and we discuss the fundamental mechanisms of charge transfer in the ultrashort time window following the impulsive excitation. When the HIOS is excited by a resonant laser pulse, the charge transfer across the interface is increased compared to the ground state but is not further enhanced by vibronic coupling. In this presentation [2] we highlight the complexity of the physics involved and demonstrate the ability of the adopted formalism to achieve a comprehensive understanding of the ultrafast charge-transfer in HIOS.

[1] J. Krumland et al., submitted (2020) arXiv:2003.08669.

[2] M. Jacobs et al., Advances in Physics: X 5, 1749883 (2020).

### **13** Switching impact of photochromic diarylethenes as self-assembled monolayer in organic light emitting diodes

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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 the functionalization of a transparent indium tin oxide (ITO) electrode with a SAM realized with a derivative of a switching molecule (diarylethene) enabling optical control of electronic properties over the electrode interface. By combining a range of various surface characterization techniques, we present a detailed picture of the SAM binding onto ITO. As a proof-of-principle, an organic light emitting 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 could be exploited for novel optoelectronic logic circuits.

### **14** Excited state charge transfer at the phthalocyanine/MoS<sub>2</sub> Interface

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Combining monolayer (ML) transition metal dichalcogenides (TMDCs) with organic semiconductors promises to improve on the individual optoelectronic properties and to add new device functionality. In such hybrid structures, energy or charge transfer can e.g. lead to an enhanced photoconductivity of the TMDC ML, thereby improving its photodetection capability. Here, we show that a 3 nm thick layer of metal-free phthalocyanine (H<sub>2</sub>Pc) not only increases but also extends the photo-response of the underlying MoS<sub>2</sub> ML. This enhancement in photoconductivity is experimentally traced back to an excited state electron transfer from the H<sub>2</sub>Pc layer to MoS<sub>2</sub>. Photoemission spectroscopy reveals that the H<sub>2</sub>Pc/MoS<sub>2</sub> system forms a robust type II interface with energy offsets on the order of 1 eV. Time resolved photoluminescence (PL) measurements unveil efficient exciton dissociation manifested by a shortening of the H<sub>2</sub>Pc PL decay time when in contact to MoS<sub>2</sub>. The charge transfer excitons at the hybrid interface dissociate into free carriers, subsequently contributing to the MoS<sub>2</sub> photoconductivity as demonstrated by photocurrent action spectroscopy. These findings show that by choice of suitable molecules new functionality can be added to TMDCs.

## 15 Fundamental properties of single-photon sources in hexagonal boron nitride

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Single-photon emitters (SPEs) in hexagonal boron nitride have proven to be bright, stable and spectrally narrow. In combination with the flexibility of the two-dimensional host material, this system is potentially suitable for integration into future quantum photonic technologies.

So far, one of the difficulties of this system is the wide spectral range in which the zero-phonon line of the individual SPEs is distributed. Although there are advances in the fabrication, individual tuning of each emitter is probably inevitable. Here, we present a method for this and demonstrate a large Stark tuning of  $(5.9 \pm 0.6)$  nm [1]. Additionally, the dipole moment and polarizability and thus the size of the SPE could be measured.

In a second experiment we investigated the spectrally dependent quantum efficiency of the SPEs by the Drexhage method [2], which is a crucial parameter for any application. This system-immanent parameter could be useful in the future to identify the atomic origin of these SPEs.

[1] N. Nikolay, N. Mendelson, N. Sadzak, F. Böhm, T. T. Tran, B. Sontheimer, O. Benson, *Phys. Rev. Appl.* 11, 041001 (2019).

[2] N. Nikolay, N. Mendelson, E. Özelci, B. Sontheimer, F. Böhm, G. Kewes, O. Benson, *Optica* 6, 1084 (2019).

## 16 Optical properties of iodoplumbate chains formed in solutions: from experiment to theory

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Solvent-solute interactions in precursor solutions play an important role in controlling the quality of solution-processed hybrid perovskites. These chemical interactions lead to the formation of a variety of polyiodide plumbates that act as building blocks for hybrid perovskites. The formation of  $[\text{PbI}_{2+n}]^{n-}$  complexes is often expected in diluted solutions of hybrid perovskites, while coordination processes occurring in concentrated solutions are not yet well understood.

In this work, we demonstrate the optical properties of the quasi-one-dimensional iodoplumbate chains  $\text{PbI}_2(\text{DMSO})_4$ ,  $\text{Pb}_2\text{I}_4(\text{DMSO})_6$ , and  $\text{Pb}_3\text{I}_6(\text{DMSO})_8$  formed in DMSO solutions at high concentration of lead iodide [1]. The increase of the length of the chain from  $\text{PbI}_2(\text{DMSO})_4$  to  $\text{Pb}_3\text{I}_6(\text{DMSO})_8$  leads to a red shift of the absorption spectrum. The structure and the optical response of iodoplumbate chains were modeled via *ab initio* many-body simulations. Through the analysis of the computed molecular orbitals, optical spectra, and electron and hole densities, we rationalize the influence of electronic hybridization between solute and solvent and the mechanisms that are responsible for the optical properties of polyiodide plumbate chains.

[1] A. M. Valencia, R. Schier, O. Shargaieva, E. Unger, and C. Cocchi (manuscript in preparation).

## 17 Evolution of pure hydrocarbon hosts for the application in universal OLEDs

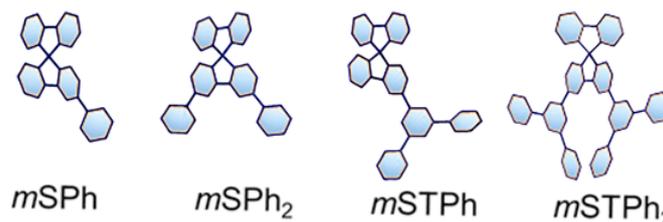
Qiang Wang<sup>1,2</sup>, Fabien Lucas<sup>2</sup>, Cassandre Quinton<sup>2</sup>, Yang-Kun Qu<sup>1</sup>, Joelle Rault-Berthelot<sup>2</sup>, Olivier Jeannin<sup>2</sup>, Sheng-Yi Yang<sup>1</sup>, Fan-Cheng Kong<sup>1</sup>, Sarvendra Kumar<sup>1</sup>, Liang-Sheng Liao<sup>1</sup>, Cyril Poriel<sup>2</sup>, Zuo-Quan Jiang<sup>1</sup>

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In the field of phosphorescent organic light-emitting diodes (PhOLEDs), designing high-efficiency universal host materials for red, green and blue (RGB) phosphors has been quite a challenge. To date, most of the high-efficiency universal hosts reported incorporate heteroatoms, which have a crucial role in the device performance. However, the introduction of different kinds of heterocycles increases the design complexity and cost of the target material and also creates potential instability in the device performance. In this work, we show that pure aromatic hydrocarbons hosts designed with the 9,9'-spirobifluorene scaffold are high-efficiency and versatile hosts for PhOLEDs. With external quantum efficiencies of 27.3%, 26.0% and 27.1% for RGB PhOLEDs respectively, this work not only reports the first examples of high-efficiency pure hydrocarbon materials used as hosts in RGB PhOLEDs but also among the highest performance reported to date for a universal host (including heteroatom-based host). This work shows that the PHC design strategy is promising for the future development of OLED industry as a high-performance and low-cost option.



## 18 Optoelectronic properties of monolayer MoS<sub>2</sub> with sulfur vacancies

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Monolayer MoS<sub>2</sub> is known to exhibit outstanding optoelectronic properties which make it a very interesting material for hybrid inorganic/organic systems [1]. However, its remarkable characteristics may be (negatively) affected by defects. Here, we study theoretically the impact of sulfur vacancies (SVs) on the opto-electronic properties of monolayer MoS<sub>2</sub>. We employ **exciting**, a full-potential all-electron DFT code [2], to perform *ab initio* calculations within many-body perturbation theory at the level of  $G_0W_0$  and the Bethe-Salpeter equation (BSE). Compared to the pristine material, the SVs tend to redshift the absorption spectrum and to decrease its intensity.

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[2] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, C. Draxl, *J. Phys.: Condens. Matter* 26, 363202 (2014).

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

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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]. We benchmark our implementation by analyzing the electric current density and the ion dynamics of Si, C, SiC, and two-dimensional BN and MoS<sub>2</sub> under the exposure to laser pulses. Our results are benchmarked against those obtained using the octopus code [3].

[1] A. Gulans et al., J. Phys.: Condens. Matter 26, 363202 (2014).

[2] G. Kolesov, et al., J. Chem. Theory Comp. 12, 466 (2015).

[3] X. Andrade et al., Phys. Chem. Chem. Phys. 17, 31371 (2015).

## 20 Waveguide mode modulation with photochromic molecules for neuromorphic computing

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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.

## 21 Individual tubular J-aggregates stabilized and stiffened by silica encapsulation

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The amphiphilic cyanine dye 3,3'-bis(3-sulfopropyl)-5,5',6,6'-tetrachloro-1,1'-dioctylbenzimidazole-carbo-cyanine (C8S3) in aqueous solution self-assembles into micrometer long double walled tubular J-aggregates with a uniform outer diameter of  $13 \pm 0.5$  nm. These J-aggregates exhibit strong exciton delocalization and migration, similar to natural light harvesting systems. However, their structural integrity and optical properties are very sensitive to their chemical environment as well as to mechanical deformation. We address this issue for their chemical and mechanical stabilization by in situ synthesis of a silica coating that leaves their structure and optical properties mostly unaltered. [1] Here, we demonstrate that the silica shell with a thickness of a few nanometers is able to stabilize the tubular J-aggregates of C8S3 against changes of pH and against drying up to vacuum conditions within an electron microscope. Dried silica-covered aggregates are brittle, as demonstrated by manipulation with a scanning force microscope on a surface. Transmission electron microscope images confirm that the thickness of the coatings of less than 5 nm is homogeneous and uniform; TEM energy dispersive X-ray and electron energy loss spectroscopy could be achieved on a scan across a single freely suspended aggregate. Such a silica shell may not only serve for stabilization but also could be the base for further functionalization of the aggregates by either chemical attachment of other units on top of the shell or by inclusion during the synthesis.

[1] Y. Qiao, F. Polzer, H. Kirmse, S. Kirstein, and J. P. Rabe, Chem. Commun. 51, 11980 (2015).

## 22 Computational characterization of defect-state lasing in hybrid plasmonic-organic micro-cavities

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Defects in photonic crystals can create high quality cavities. We investigate a lasing resonator consisting of two one-dimensional distributed Bragg reflectors (DBRs). An in-plane patterning can further facilitate a three-dimensional mode confinement.

We here present how to utilize the resulting resonator modes to achieve controllable lasing thresholds of an experimental realization of such a setup. The DBRs consist of SiO<sub>2</sub> and TiO<sub>2</sub> layers, while the cavity includes a regular one-dimensional silver grating including a defect. The defect width allows controlling the lasing of the incorporated Alq<sub>3</sub>/DCM dye under focused beam excitation.

To compute the lasing thresholds, we use the discontinuous Galerkin time domain method [1], in order to solve Maxwell's equations accompanied with the rate equations for the four-level system [2] that models the organic dye. Full access to the fields provides a deeper insight into the nonlinear time-dynamics of the system.

[1] K. Busch, M. König, J. Niegemann, Laser & Photonics Reviews 5, 773 (2011).

[2] S.-H. Chang and A. Taflove, Opt. Express 12, 3827 (2004).

## 23 Challenges in evaporation of organic diradicals

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After previously demonstrating the possibility of evaporating purely organic diradicals preserving the radical character [1], we now investigate the evaporation of several diradicals that were thought to be impossible to evaporate because of their high reactivity. For this we investigate diradical thin films with x-ray photoelectron spectroscopy, near-edge x-ray absorption fine structure spectroscopy, and atomic force microscopy.

Our results show that the evaporation parameters are characterized by a very narrow temperature window between successful evaporation and degradation of the radical and that film properties of diradicals are defined by the bulk formation energy, i.e. the intermolecular forces, resulting in low adhesion to the substrate with consequent quick desorption with heating, predominantly Volmer-Weber-like island growth [2] and the onset of thermal degradation. Furthermore, the high reactivity of the diradicals leads to decreased film stability against exposure to air, and even inert gases, which impedes ex-situ experiments like electron paramagnetic resonance spectroscopy.

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[2] T. Junghoefer, N. M. Gallagher, K. Kolanji, E. Giangrisostomi, R. Ovsyannikov, T. Chassé, M. Baumgarten, A. Rajca, A. Calzolari, M. B. Casu, submitted.



## Poster Session II

## 24 Benchmarking electric field responses in all-electron electronic structure calculations

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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 poster, we discuss the implementation of electronic polarization and its response to electric fields in periodic systems 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]. 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 accurate values of Born effective charges for different bulk and 2D transition metal dichalcogenide (TMDCs) materials using hybrid exchange correlation functionals. The second application involves the simulation of infrared and Raman spectra of bulk and 2D TMDCs, as well as model simulations of enhanced Raman spectra obtained from local electronic-density responses of organic molecules on inorganic surfaces.

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[2] H. Shang et al., New J. Phys. 20, 073040 (2018).

[3] V. Blum et al., Comp. Phys. Comm. 180, 2175 (2009).

## 25 Viewing singlet fission in momentum space

Alexander Neef<sup>1</sup>, Samuel Beaulieu<sup>1</sup>, Shuo Dong<sup>1</sup>, Tommaso Pincelli<sup>1</sup>, Sebastian Hammer<sup>2</sup>, Jens Pflaum<sup>2</sup>, Martin Wolf<sup>1</sup>, Laurenz Rettig<sup>1</sup>, Ralph Ernstorfer<sup>1</sup>

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Optical transitions in closed-shell systems can only lead to excited singlet states due to the lack of spin transfer. In certain molecular systems, however, the coupling between excited and ground state singlets creates two triplets, in a spin-allowed process called singlet fission. The molecular crystals of pentacene and rubrene are prototypical singlet fission materials. For those two systems, we report singlet fission dynamics and momentum-space signatures of the involved transient states (see Fig. 1) investigated with time- and angle-resolved photoemission spectroscopy based on a high-repetition rate extreme ultraviolet laser and a momentum microscope spectrometer.

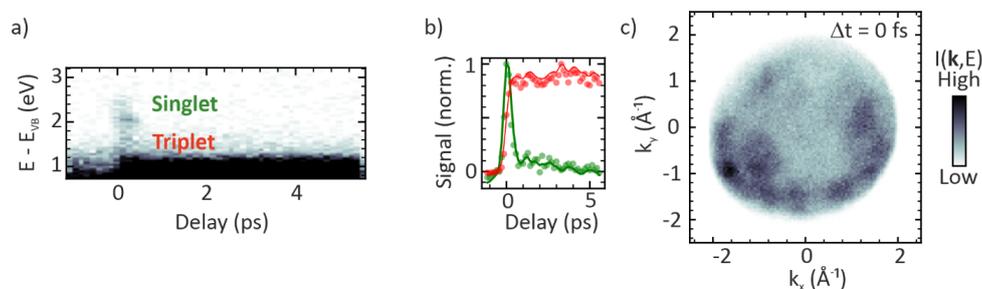


Fig. 1: a,b) Electron dynamics in pentacene. c) Momentum-space signature effect of the triplet state in pentacene.

## 26 Electronic properties of hybrid monolayer TMDC-conjugated molecule interfaces from first principles

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In view of unraveling the fundamental mechanisms of laser-induced dynamics in hybrid inorganic/organic interfaces, we investigate the electronic structure of different combinations of transition metal dichalcogenide (TMDC) monolayers  $\text{MX}_2$  (where  $\text{M}=\text{Mo}/\text{W}$  and  $\text{X}=\text{S}/\text{Se}$ ) interfaced with planar C-conjugated molecules such as pyrene and perylene. We analyze the electronic bands of these systems at different molecular concentrations. Using the effective band structure (EBS) approach, we are able to unfold the bands of the hybrid in the Brillouin zone of the TMDCs and, thus, to disclose the electronic interactions with the molecular adsorbates in a transparent way. We additionally characterize the energy level alignment of these interfaces and find that this property is essentially determined by the chalcogen atom only: Regardless of the adsorbed molecules and their concentration, interfaces including selenide monolayers exhibit a type-I line-up, whose containing sulfides form a type-II interface. Remarkable hybridization effects in the valence region are obtained for pyrene adsorbed on  $\text{MoSe}_2$ . These findings offer promising perspectives for further investigations on the excited-state dynamics in these materials.

## 27 Nonmagnetic single-molecule spin-filter based on quantum interference

Atindra Nath Pal<sup>1,2</sup>, Dongzhe Li<sup>3</sup>, Soumyajit Sarkar<sup>4</sup>, Sudipto Chakrabarti<sup>1</sup>, Ayelet Vilan<sup>1</sup>, Leor Kronik<sup>4</sup>, Alexander Smogunov<sup>5</sup>, Oren Tal<sup>1</sup>

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The field of spintronics is based on spin-polarized currents in which the current is dominated by one electronic spin type. Spin polarized currents are practically produced by spin injection from magnetic materials or by separating spin currents with the aid of magnetic fields. Here, we show that spin-polarized currents can be generated at the single-molecule scale without magnetic components or magnetic fields. Specifically, shot noise measurements detect spin polarized currents in single molecule junctions based on silver electrodes bridged by a vanadocene molecule with total spin  $S=3/2$ . In contrast, the electronic transport through similar junctions based on ferrocene with  $S=0$  do not show any indication for spin polarized currents. Transport calculations compared with conductance and shot noise measurements reveal a mechanism based on spin-dependent quantum interference at the  $S=3/2$  single molecule junction that can lead to almost 100% spin filtering. These findings pave the way for spintronic manipulations by quantum interference at the molecular scale.

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[2] A. N. Pal, T. Klein, A. Vilan, O. Tal, Beilstein J. Nanotechnol. 9, 1471 (2018).

## 28 Post rupture evolution and jump to molecular contact in single molecular junction

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As the size of the transistor is approaching the few nanometers limit, there has been a surge of interest in understanding the electrical and thermal properties at the atomic limit. The metal-molecule interface plays a key role in determining the transport properties through a molecular junction. The formation of contacts between two metallic surfaces often involves a jump from tunneling to the contact regime. It was shown that the local electrode configuration and material composition before contact primarily determine the presence or absence of a jump [1]. In the case of molecular junctions, however, jump to contact is rarely observed mostly due the fact that molecules tend to lay flat on the surface after the breaking process [2]. Here, we present a systematic investigation of the formation of molecular contacts through mechanically controlled break junction technique (MCBJ) at ambient conditions. Two structurally different molecules with similar anchoring group, 4, 4' bipyridine (BPY) and 2, 2' bipyridine have been studied with gold as electrodes. In both cases, we observe formation of molecular junction in the breaking traces, consistent with previous reports [3]. A closer look at the closing traces reveals that 4,4' BPY forms molecular junctions via a conductance jump from the tunnelling regime, whereas, 2,2' BPY does not form a clear molecular junction showing molecular assisted tunnelling till the formation of metallic contact. Through a combination of statistical analysis of the experimental data, along with, molecular dynamics and first-principles electronic structure calculations the mechanism behind the junction formation in these two different cases is unravelled.

[1] C. Untiedt et al., Phys. Rev. Lett. 98, 1 (2007).

[2] A. Vladyka et al., Nat. Commun. 10, 1 (2019).

[3] S. Y. Quek et al., Nat. Nanotechnol. 4, 230 (2009).

## 29 Excited state dynamics of unsubstituted terrylene, a textbook molecule

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In hybrid solar cells, the separation of the electron-hole pairs after photogeneration is a key aspect of the light harvesting functionality. 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). The steady state absorption and emission of terrylene molecules in solution show mirrored lineshapes characteristic of Frank-Condon coupling to a single vibrational mode. 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]. The measurement of the thin films shows, in addition to the known longer dynamics, spectral components with dynamics three orders of magnitude faster than in the single molecule. Studying the physical mechanisms arising from these aggregates is challenging but necessary to exploit the excitations of terrylene in Hybrid systems.

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### **30 Theory of short wavelength spectroscopy of two-dimensional HIOS: Exciton dynamics in tr-ARPES and X-ray response**

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Time and angle resolved photoemission spectroscopy (tr-ARPES) exploits the photoelectric effect using extreme ultraviolet light and allows to investigate ultrafast dynamics of hybrid electronic excitations directly in momentum space [1]. However, materials such as monolayer transition-metal dichalcogenides (TMDC) or hybrid interfaces exhibit tightly bound excitons, which dominate their optical properties. We develop a theory of excitonic time and angle resolved photoemission spectroscopy, showing that tr-ARPES is able to directly access excitons and probe their dynamics throughout the Brillouin zone [2,3]. We discuss the extension of our theory to functionalized TMDCs, where a more complex exciton dynamics take place due to spatial energy and charge transfer [4].

A second spectroscopic method exploiting high energy radiation is X-ray absorption spectroscopy (XAS). Here, deep-core electrons are excited into conduction band states and the ionization continuum leading to core specific edges in the absorption spectrum. We present a theoretical framework for XAS for atomically thin two-dimensional materials. Using a tight binding model and nonlocal light-matter interaction we analyze the characteristic behavior of XAS spectra [5].

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### **31 Modulating guest uptake in core-shell MOFs with visible light**

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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]

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### **32** Structural dynamics of pentacene single crystals and MoS<sub>2</sub>/pentacene heterostructures

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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 MoS<sub>2</sub>/pentacene heterostructure, with the ultimate aim of revealing the dynamics of interfacial vibrational energy transfer.

### **33** In situ investigation of the Cu/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> interface in perovskite device

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In this study, we constructed a pristine Cu/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>/NiOx/indium tin oxide (ITO) solar cell device. The initial power conversion efficiency (PCE) of the pristine device is 8.8% and remains almost constant over long-time testing under the standard operating conditions (49 days). In order to fundamentally understand this extraordinary long-term device stability, the electronic properties and chemical stability of the Cu/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> interface were comprehensively investigated in-situ by a combination of X-ray photoemission spectroscopy (XPS), synchrotron radiation photoelectron spectroscopy (SRPES) and ultraviolet photoemission spectroscopy (UPS). In addition, scanning electron microscopy (SEM) was used to check the growth of Cu deposited on the perovskite surface. The results show that no chemical reaction between Cu and the perovskite takes place which may lead to an outstanding long-term stability. Moreover, an interface dipole of 0.45 eV and 0.15 eV upward band bending at the Cu/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> interface were found. This study demonstrates that Cu is a promising candidate to be employed as a metal electrode for perovskite solar cells.

### **34 Structural and electronic properties of F6-TCNNQ on monolayers of MoS<sub>2</sub> investigated by STM/AFM**

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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 MoS<sub>2</sub> on a metal substrate, 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.

[1] S. Park, T. Schultz, X. Xu, B. Wegner, A. Aljarb, A. Han, L.-J. Li, V.C. Tung, P. Amsalem, N. Koch, *Commun. Phys.* 2, 109 (2019).

### **35 Donor–acceptor dihydropyrenes switchable with near-infrared light**

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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  $\pi$ -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 utilization of these donor-acceptor DHPs allows efficient photoswitching induced by NIR light, which renders them attractive for various applications.[2]

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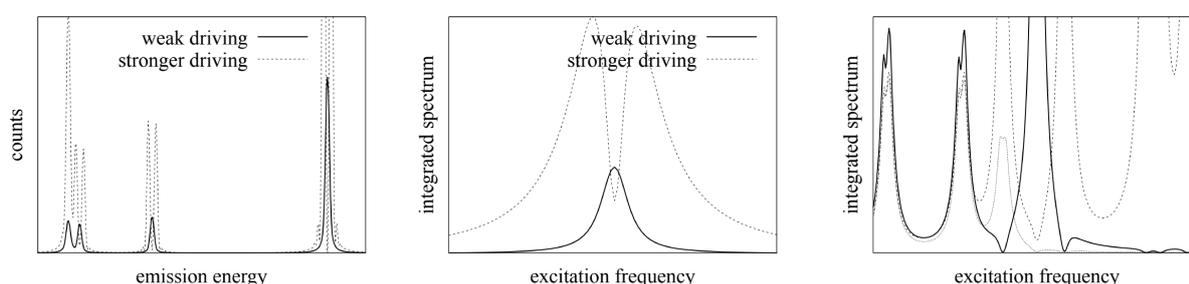
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### 36 Anticrossing effects in photoluminescence excitation spectroscopy of quantum dots

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A detailed understanding of the energy levels of confined carriers in Quantum Dots, and the interactions between them, is essential for implementing potential applications. In this context, photoluminescence excitation (PLE) spectroscopy [1] has become a widely applied experimental technique. We provide general theoretical explanations for the appearance of anticrossing-dips in respective spectra, in a phenomenological master equation approach.



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### 37 Local chiral sensors for HIOS from self-assembled plasmonic nano-antenna-waveguide structures

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Composition, structure and orientation on the nano-scale are essential properties, which define if a macroscopic HIOS device will hold its promises. Confining light to this scale is achieved through usage of plasmonic resonances of metal nanoparticles. Besides strength and direction of these fields, polarization is a vital probe for orientation, especially in chiral environments. Structural chirality in HIOS comes into play when one of the components is chiral (e.g. organic stereoisomers), but can also be a particular consequence of the whole system (e.g. contorted organic layers on an inorganic crystal).

We will present our experimental findings studying self-assembled systems of plasmonic silver nanowire waveguides[1] coupled to nanoantennas. Depending on the handedness of incident light focused down to the antenna, we detect directed plasmon excitation along the waveguide by the fluorescence of embedded PDI molecules[2]. This mimics the case when the chirality of a sample is probed locally by the plasmonic hotspot between nanoantenna and waveguide. Realizing coupling via inorganic (magnetic or chiral) scatterers, our system becomes not only a sensor, but a HIOS itself.

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[2] M. Rothe, Y. Zhao, J. Müller, G. Kewes, C. Koch, Y. Lu, O. Benson, submitted (2020).

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

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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 electron or hole transport materials. 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 MoS<sub>2</sub> combined with the hole transport molecule  $\alpha$ -NPD, we find that the dynamics of the TMDC excitons is largely governed by the trapping and recombination of charges on the MoS<sub>2</sub> layer, while we also resolve a long-lived signal which we assign to charge separation. In line with recent experiments on MoS<sub>2</sub>/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.

[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).

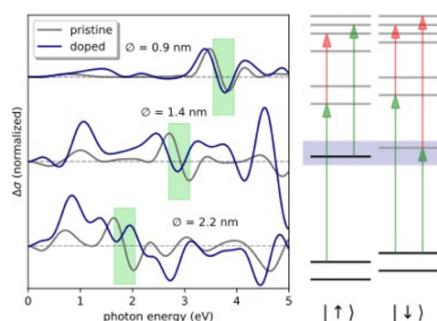
### 39 Photoinduced electron dynamics of N-doped graphene quantum dots

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Understanding how doping influences the photoinduced dynamics in graphene quantum dots (GQDs) is of paramount importance to understand and tailor the linear and non-linear optical response of these systems in optoelectronic applications. In the framework of real-time time-dependent density functional theory (RT-TDDFT), we investigate the time-resolved photoinduced electron dynamics of pristine and N-doped hexagonal GQDs with both zigzag and armchair edges up to 4 nm in size. Our results show that the presence of a single N impurity brings about substantial effects on the optical response both in the linear and in the non-linear regime. On the one hand, doping breaks both the orbital and the spin degeneracies of the GQDs and it activates symmetry-forbidden optical excitations within the optical gap. On the other hand, N-doping strongly affects the transient absorption spectra (TAS) by introducing an enhancement and a broadening of the excited state absorption below the pump frequency, due to the presence of gap states which mediate the activation of a higher number of allowed transitions.



## 40 Electronic and optical properties of $\text{Na}_2\text{KSb}$ and $\text{NaK}_2\text{Sb}$ from *ab initio* many-body theory

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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 study, we investigate from first principles, in the framework of density-functional theory and many-body perturbation theory, the electronic and optical properties of  $\text{Na}_2\text{KSb}$  and  $\text{NaK}_2\text{Sb}$ . This approach has been already successfully adopted, in conjunction with experiments, to shed light on the intrinsic properties of Cs-based alkali-antimonides [2]. The analysis of band structures and densities of states indicate that both materials are characterized by a direct quasi-particle gap of the order of 1.5 eV. The lowest-energy excitations exhibit binding energies of 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  $\text{Na}_2\text{KSb}$  and  $\text{NaK}_2\text{Sb}$  and are expected to stimulate further research on multi-alkali antimonides.

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[2] C. Cocchi, S. Mistry, M. Schmeißer, R. Amador, J. Kühn, T. Kamps, Sci. Rep. 9, 18276 (2019).

[3] R. Amador and C. Cocchi, to be submitted (2020).

## 41 Electronic structure of BCF-doped oligothiophenes from *Ab initio* many-body theory

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Lewis acids like tris(pentafluorophenyl)borane (BCF) offer promising routes for efficient p-doping of organic semiconductors. The intriguing experimental results achieved so far call for a deeper understanding of the underlying doping mechanisms. To investigate these processes on a microscopic level, we model donor/acceptor adducts as bimolecules *in vacuo* and investigate their electronic and optical properties from first principles by means of density-functional theory and many-body perturbation theory. We consider donor/acceptor complexes formed by BCF doping quarterthiophene (4T). For reference, hexafluorobenzene ( $\text{C}_6\text{F}_6$ ) and  $\text{BF}_3$  are also investigated as dopants for 4T. In the ground-state, we find negligible charge-transfer and frontier states either segregated on the opposite sides of the interface (4T:BCF) or localized on the donor (4T: $\text{BF}_3$  and 4T: $\text{C}_6\text{F}_6$ ). In the optical spectrum of 4T:BCF, a charge-transfer excitation appears at the lowest energy, corresponding to the transition between the frontier states, which exhibit very small but nonvanishing wave function overlap. In the other two adducts, the absorption is given by a superposition of the features of the constituents. Our results [1] clarify that the intrinsic electronic interactions between donor and acceptor are not responsible for the doping mechanisms induced by BCF and related Lewis acids. Extrinsic factors, such as solvent-solute interactions, intermolecular couplings, and thermodynamic effects, have to be systematically analyzed for this purpose.

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## **42** Direct observation of conductive polymer induced inversion layer in n-Si and correlation to solar cell performance

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Heterojunctions formed by ultrathin conductive polymer (PEDOT:PSS) films and n-type crystalline silicon were investigated by photoelectron spectroscopy. [1] By diluting the original PEDOT:PSS solution and increasing the spin-coating speed, a series of PEDOT:PSS thin films with the thicknesses down to 5 nm were achieved on n-Si substrates. Large shifts of Si 2p core levels upon PEDOT:PSS deposition provide direct evidence that a dopant-free p-n junction is formed within Si. Among the investigated PEDOT:PSS formulations, the largest induced band bending within Si (0.71 eV) is found for PH1000 (high PEDOT content) combined with a wetting agent and dimethyl sulfoxide (DMSO). Without DMSO, the induced band bending is reduced, as is also the case with a PEDOT:PSS (AI 4083) formulation with higher PSS content. Moreover, the addition of DMSO improves the interface between PEDOT:PSS and n-Si, as reflected by the performance of PEDOT:PSS/n-Si solar cells, and the formulation PH1000 with DMSO yielded the largest Voc (0.64 V). By comparing PEDOT:PSS/n-Si solar cells with MoOx/n-Si cells, it becomes apparent that a large contact-induced band bending does not necessarily lead to a high Voc. Adequate passivation of the silicon surface to decrease recombination and high conductivity of the covering layer are also needed to achieve high PCE devices.

[1] R. Wang, N. Koch et al., *Adv. Funct. Mater.* 30, 1903440 (2020).

## **43** Non-linear cavity QED effects in dissipative resonators using coupled quasinormal modes

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The interaction of light and matter in dissipative nanostructures has become an important topic in quantum optics and plasmonics, since it offers a variety of applications, such as lasing/spasing and non-classical light generation. Using a recent developed quantization scheme [1] for three-dimensional open resonators on the basis of quasinormal modes (QNMs) [2] with complex eigenfrequencies, we explore the higher rungs of the Jaynes-Cummings ladder in a plasmonic-photonic crystal cavity coupled to a quantum emitter. On the basis of a generalized input-output theory for QNMs [3], we derive quantum correlations of the output field using the two-QNM master equation and compare the results to a phenomenological dissipative Jaynes-Cummings model.

[1] S. Franke, S. Hughes, M. K. Dezfouli, P. T. Kristensen, K. Busch, A. Knorr, M. Richter, *Phys. Rev. Lett.* 122, 213901 (2019).

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## 44 Very high photoresponse from a few layered MoS<sub>2</sub> transistor

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Semiconducting, two-dimensional molybdenum disulfide (MoS<sub>2</sub>) is considered to be a promising new material<sup>1</sup> for high sensitive photodetection [2], because of its atomically thin profile and favorable bandgap. Monolayer MoS<sub>2</sub> possesses direct optical bandgap (~1.8 eV), however, relatively lower absorption of incident light due to its atomic thickness limits the device performance. Here, we present systematic transport data from a few layered (~3-4) MoS<sub>2</sub> field effect transistor with a high electrical on/off ratio (~10<sup>4</sup>). The device shows a huge photoresponse under optical illumination ( $\lambda$ ~633 nm) with a responsivity closed to ~10<sup>5</sup>-10<sup>6</sup>, being one of the highest for few layered devices. We plan to improve the device performance and detection range by creating hybrid with other 2D/0D TMD materials.

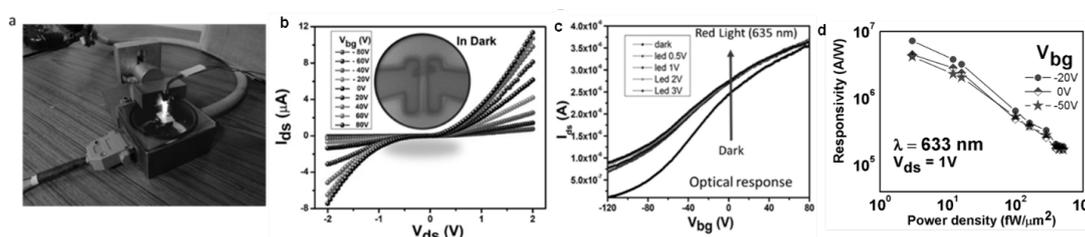


Fig. a) Optoelectronic transport measurement set up, (b) I-V characteristics at different gate voltages for a two terminal few layered MoS<sub>2</sub> transistor. Inset shows the device image. (c)  $I_{DS}$ - $V_{bg}$  characteristics in dark and, in presence of red light, showing a significant photo response. (d) Calculated Responsivity plotted as a function of optical power for three different gate voltages.

[1] Radisavljevic et al., Nat. Nanotechnol. 6, 147 (2011).

[2] Zongyou Yin et al., ACS Nano 6, 74 (2012).

## 45 Dynamic screening of quasiparticles in WS<sub>2</sub> monolayers

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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 WS<sub>2</sub> monolayers on SiO<sub>2</sub>: 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.

The main observation is a pump photon energy-dependent blue/red shift of the neutral exciton for resonant/above-resonance pumping, respectively. Both, photoexcited excitons and quasi-free carriers screen the Coulomb interaction, leading to a weaker/stronger renormalization of the quasi-free-particle band gap compared to the dynamic screening-induced reduction of the exciton binding energy. The relative interplay between these two effects explains the observed blue/red shift crossover.

Using a simple rate equation model, it is possible to, for instance, extract exciton formation and decay times from the multiexponential dynamics of the exciton resonances.

### **46** In-situ evaporation of molecular dopants on monolayer/bilayer TMDCs

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We investigate excitonic physics arising from controlled evaporation of molecules (F4TCNQ, TTF) on the surface of various TMDCs, inside the cryostat with optical access at room and low temperatures. Molecules are deposited from the on-chip lithographically made evaporator, placed close to the device with monolayer/bilayer TMDC flake. The direct n or p type doping effect of the molecules can be achieved, with controllable doping dose. Ultimately we plan to find conditions for the low-density molecular submonolayer. This hybrid inorganic-organic system is promising for discovering effects of trapping excitons with localized electric field, and revealing dark excitons.

## Contact

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