

Optoelectronic Processes at Nanostructured Interfaces

763. WE-Heraeus-Seminar

14 – 16 March 2022

hybrid

at the Physikzentrum Bad Honnef, Germany

**WILHELM UND ELSE
HERAEUS-STIFTUNG**



Introduction

The Wilhelm und Else Heraeus-Stiftung is a private foundation that supports research and education in science with an emphasis on physics. It is recognized as Germany's most important private institution funding physics. Some of the activities of the foundation are carried out in close cooperation with the German Physical Society (Deutsche Physikalische Gesellschaft). For detailed information see <https://www.we-heraeus-stiftung.de>

Aims and scope of the 763. WE-Heraeus-Seminar:

The growing demand for higher computing power, more selective sensing, and alternative energy production requires new generations of materials for future optical and electrical devices with higher efficiencies and lower costs. The development of such devices is expected to enable a broad range of electronic applications amongst which are LEDs both for lighting and for displays, batteries and capacitors, highly selective catalysts and electrocatalysts, sensors and photodetectors, and many more. For that purpose, nanostructured materials can be exploited in solution or in the solid state, for instance as thin films, either pure or as combinations by self-assembly. Due to the ongoing miniaturization and the use of nanomaterials and with this the increased surface-to-volume ratio the interfaces gain more and more relevance. Eventually, an understanding of the materials' interface properties is essential for their application in high-performance devices. Further, tailoring and controlling the electronic structure at the interface has a profound impact on their optoelectronic properties. In this WE-Heraeus Seminar, leading experts from synthetic chemistry (providing the materials), experimental physics (characterizing the materials) and computational material science (tracing the mechanisms) will address the problems, challenges and opportunities in the field of nanostructured interfaces for optoelectronics, highlight perspectives for future applications, report on new possibilities in synthesis and characterization, inspire novel research directions and foster collaborative efforts amongst the participants.

Scientific Organizers:

Prof. Christian Klinke

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Introduction

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Registration:

Elisabeth Nowotka (WE Heraeus Foundation)
at the Physikzentrum, reception office
Sunday (17:00 h – 21:00 h) and Monday
morning

Program

Sunday, 13 March 2022

17:00 – 20:00 Registration

18:00 *BUFFET SUPPER and informal get-together*

Monday, 14 March 2022

08:00 *BREAKFAST*

08:50 – 09:00 Scientific organizers **Welcome words**

09:00 – 09:50 Thomas Frauenheim **Theory of 2D materials**

09:50 – 10:10 Dmitry Baranov **The good, the bad, and the ugly transformations of cesium lead bromide nanocrystals**

10:10 – 10:30 Saskia Fiedler **Cathodoluminescence spectroscopy of silicon nanoparticles**

10:30 – 11:00 *COFFEE BREAK*

11:00 – 11:50 Bettina Lotsch **Interface design across the scales in molecular and hybrid solids**

11:50 – 12:10 Henk Stoof **Topological Wannier excitons in Bismuth chalcogenides nanosheets**

12:10 – 12:30 Laurens Siebbeles **Observing quantum-confinement effects on the in-plane translational motion of excitons in CdSe nanoplatelets**

12:30 – 12:45 **Conference photo**

12:45 *LUNCH*

Program

Monday, 14 March 2022

14:10 – 15:00	Tobias Kipp	Colloidal quantum nanowires: Structural, optical, and electronic properties
15:00 – 15:20	Vincent Mauritz	Gaining insights into the ABX₃ chalcogenide material BaTiS₃ for NIR applications
15:20 – 15:40	Sushant Ghimire	High quantum yield, broadband, and delayed emission in two-dimensional tin iodide perovskite nanosheets
15:40 – 17:30	Poster session <u>on site</u> and <i>COFFEE BREAK</i>	
17:30 – 18:30	Hilmi Volkan Demir	Semiconductor nanocrystal optoelectronics: From advanced heterostructures to oriented self-assemblies of colloidal quantum wells <i>PLUS:</i> Discussion on the future of nanoelectronics in respect of the day's subjects
19:00	HERAEUS DINNER <i>(social event with cold & warm buffet with complimentary drinks)</i>	

Program

Tuesday, 15 March 2022

08:00	<i>BREAKFAST</i>	
09:00 – 09:50	Julia Stähler	Dynamic screening of quasiparticles in WS₂ monolayers
09:50 – 10:10	Paul Mulvaney	Spectroelectrochemistry of CdSe quantum dots
10:10 – 10:30	Tassilo Naujoks	Quantum efficiency enhancement of Lead-Halide Perovskite nanocrystal LEDs by organic Lithium salt treatment
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:50	Emmanuel Lhuiller	By design light matter interaction in nanocrystal array, a step toward active nanophotonics
11:50 – 12:10	Yan B. Vogel	Charge percolation in QD–molecule assemblies
12:10 – 12:30	Lars Frederik Klepzig	Colloidal 2D PbSe nanoplatelets with efficient emission reaching the Telecom O-, E- and S-band
12:30	<i>LUNCH</i>	

Program

Tuesday, 15 March 2022

14:00 – 14:50	Jannika Lauth	A colloidal 2D semiconductors covering visible to telecom window wavelengths - combining chemistry and spectroscopy for innovative optoelectronics and photonic quantum technologies
14:50 – 15:10	Francisco M Gómez-Campos	Electronic structure of InAs quantum dot solids: Influence of dimensionality and stoichiometry
15:10 – 15:30	Jia Grace Lu	Optoelectronic processes in low dimensional systems
15:30 – 17:30	Poster session <u>on site</u> and <i>COFFEE BREAK</i>	
17:30 – 18:30	Andres Castellanos-Gomez	Controlling the metal/semiconductor interface in 2D-dimensional based devices <i>PLUS:</i> Discussion on the future of nanoelectronics in respect of the day's subjects
18:30 – 18:45	Stefan Jorda	About the Wilhelm and Else Heraeus-Foundation
19:00	<i>DINNER</i>	

Program

Wednesday, 16 March 2022

08:00	<i>BREAKFAST</i>	
09:00 – 09:50	Alexander Holleitner	Femtosecond electronics across nanostructured interfaces
09:50 – 10:10	Karen Schäfer	Modelling mechanical properties of Gold nanoparticle arrays with molecular dynamics
10:10 – 10:30	Rostyslav Lesyuk	Role of Mn–Mn coupling in photoluminescence kinetics of doped ZnS nanoplatelets
10:30 – 11:00	<i>COFFEE BREAK</i>	
11:00 – 11:50	Jana Zaumseil	Tailored Interfaces with and defects in single-walled carbon nanotubes
11:50 – 12:10	Sergio Puebla	In-plane anisotropic properties of two-dimensional MoO₃
12:10 – 12:30	Dipankar Bain	Aggregation induced emission: A novel strategy for lighting metal nanoclusters
12:30 – 12:45	Scientific organizers	Concluding keynote <i>PLUS:</i> Poster prizes
12:45	<i>LUNCH</i>	

End of the seminar and departure

NO DINNER for participants leaving on Thursday morning

Posters

Posters

- Shaimaa Abdalbaqi **Coupled organic-inorganic nanostructures photodiodes using single and heterostructure types of ligands**
- Artsiom Antanovich **Alloyed CdSe_xS_{1-x} nanoplatelets with continuously tunable blue-green emission**
- Aswin Asaithambi **Exciton energy funneling in perovskite-TMDC (0D-2D) hybrid system**
- Dina Atwa Khalil **Optical, structural and optoelectronic properties of pulsed laser deposition PbS thin film.**
- Raktim Baruah **Thin films via deposition of colloidal nanocrystals for high order harmonic generation**
- Leon Biesterfeld **Surface treatment of colloidal 2D PbSe NPLs for emission enhancement at Telecom wavelengths**
- Ankita Bora **Controllable doping of semiconductor nanocrystals via cation exchange**
- Onur Çakıroğlu **Motorized stage allowing improvements in strain engineering in 2D materials**
- Mariarosa Cavallo **Split-gate photodiode based on graphene/HgTe heterostructure with a few nanosecond photoresponse**
- Nicola Curreli **Depletion layer engineering in core-shell metal oxide nanocrystals**
- Katharina Dehm **Low-toxicity and sustainable chalcogenide materials for photovoltaic application**
- Mareike Dittmar **Synthesis and characterization of hybrid semiconductor-metal nanostructures for photocatalytical applications**
- Ningyuan Fu **Optimized cation exchange for Mercury chalcogenide 2D nanoplatelets**

Posters

- Michele Ghini **Light-driven energy storage solutions based on the coupling between metal oxide nanocrystals and 2D materials**
- Johannes Gröbmeyer **Towards tunnel gaps for nanoscale on-chip ultrafast photoemission currents**
- Udara Bimendra Gunatilake **Magneto assisted underwater bubble manipulation**
- Philipp Haizmann **Impact of the ligand shell on structural change and decomposition of all-inorganic mixed-halide perovskite (CsPbX₃) nanocrystals under X-ray illumination [1]**
- Nabila Jarmouni **Synthesis, optical and structural properties of lead bromide perovskite nanocrystals for lighting emitters devices**
- Adrien Khalili **Expansion of the InGaAs spectral response with HgTe nanocrystals**
- Krishan Kumar **Ultrafast transient pump-pump-probe spectroscopic investigations on seeded nanorods**
- Sanaa Lahlali **Analysis of the conduction mechanism of the new nanomaterial Cu₂SnS₃ compound synthesized by hydrothermal route**
- Sergey Lavrentyev **Time- and frequency-domain opto-electrical measurements on graphene at THz frequencies**
- Daniel Lengle **Cation exchange on single semiconductor**
- Hao Li **Strongly anisotropic strain-tunability of excitons and Raman shift in exfoliated ZrSe₃ and ReS₂**
- Lina Makke **How does surface chemistry control the shape of semiconductor nanoplatelets?**

Posters

- Mark Mangnus **Finite-size effects on energy transfer between dopants in nanocrystals**
- Georg Moethrath **Nanowire based photovoltaic devices**
- Abdo Mohsen **2D/1D MoS₂/TiO₂ heterostructure with wavelength-dependent charge transfer pathway for selective photocatalytic CO₂ reduction**
- André Niebur **Ultrafast interactions in dual-plasmonic core-shell Au@CuS nanoparticles**
- Oussama Oulhakem **The effect of water intercalation into tungsten trioxide structure on photocatalytic properties: connectin between crystallographic structure and electronic properties**
- Prabhat Ranjan **Computational study of chalcopyrite-type nanomaterials for solar cell applications**
- Boutaina Rezki **Alkali metal modified fluorapatite as promising catalysts for biodiesel production**
- Andrea Rubino **Indium tin oxide (ITO) nanocrystals photo-doping: exploiting multiple-charge processes**
- Dominik Rudolph **Transient absorption spectroscopy of colloidal 2D transition metal dichalcogenides (TMDCs) at cryogenic temperatures**
- Olga Smirnova **Photoluminescence polarization of an ensemble of arbitrarily oriented colloidal nanoplatelets**
- Fabian Strauß **Exploring the limits of neat MoS₂ photodetectors**
- Onno Strolka **Insights into colloidal 2D MoS₂ nanosheet formation**
- Sander Vonk **Enormous artifacts in luminescence nanothermometry**
- Moritz Wehrmeister **Kelvin probe force microscopy of nanostructures**

Abstracts of Talks

(in alphabetical order)

Aggregation Induced Emission: A Novel Strategy for Lighting Metal Nanoclusters

Dipankar Bain and Amitava Patra

Institute of Nano Science and Technology, Mohali, India

Metal nanoclusters (NCs) are ultrasmall size metal nanoparticles (typical core size < 2 nm) which connect the gap between plasmonic NPs and atoms.^{1, 2} Metal NCs are emerged as a versatile photonic material in biomedical fields, including bioimaging, biosensing, intracellular detection, and therapeutics. The emergence of quantum effect NCs induces molecular-like electronic transitions between discrete energy levels giving rise to unprecedented chemical and physical properties. Among them, photoluminescence (PL) has become the center of attention, though the exact mechanism is not fully understood yet. However, one of the major concerns for NCs is their low quantum yield (QY) which limits their practical applications in bio-imaging and light-emitting diodes (LEDs). Aggregation-induced emission (AIE), is an efficient strategy that has gained significant attention for luminescence enhancement compared to the other methods.^{3, 4} In the last decade, several groups have achieved highly luminescent thiolate protected MNCs by using the AIE strategy. It is worth mentioning that the exact mechanism of PL enhancement in these AIE-type NCs is not still fully understood. There is various driving force that plays a major role in the aggregation of NCs including the intercluster attraction force and metallophilic interactions involving the surface ligands or surface motifs. The pHs, solvents, temperature, metal ions, lights, biomolecules, and polymer matrix can control the aggregation of MNCs. Intramolecular motions like rotation and vibration associated with the surface ligands regulate the radiative and nonradiative relaxations and therefore, by controlling the ligand's motions photoemission can be enhanced. A detailed theoretical and experimental investigation is needed to understand the mechanism of photoemission enhancement in AIE-type NCs systems. The design of highly luminescent AIE-type NCs are beneficial for many applications including bioimaging and LEDs.

References

- [1] S. Maity, D. Bain and A. Patra, *Nanoscale*, **11**, 22685-22723 (2019).
- [2] D. Bain, S. Maity and A. Patra, *Phys. Chem. Chem. Phys.*, **21**, 5863-5881 (2019).
- [3] D. Bain, S. Maity and A. Patra, *Chem. Communi.*, **56**, 9292-9295 (2020).
- [4] S. Chakraborty, D. Bain, S. Maity, S. Kolay and A. Patra, *J. Phys. Chem. C*, **126**, 2896-2904 (2022).

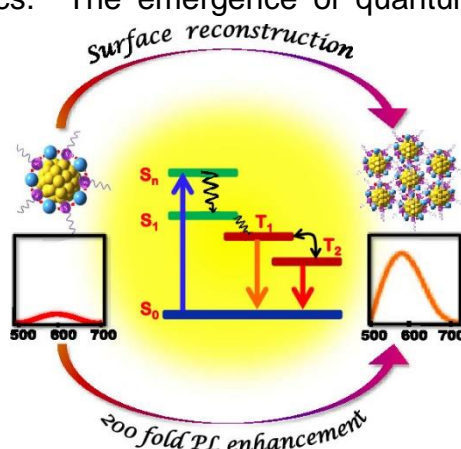


Figure.1. Schematic illustration of photoemission origin in AIE-type nanoclusters.

The Good, the Bad, and the Ugly Transformations of Cesium Lead Bromide Nanocrystals

D. Baranov¹ and L. Manna¹

¹*Italian Institute of Technology, Genova, Italy*

Colloidal metal halide nanocrystals took materials science by storm since their emergence several years ago. Exemplified by cesium lead halide perovskites, such materials show bright photoluminescence and are cheap and deceptively simple to make. These characteristics spurred applications of colloidal perovskites as low-cost phosphors, light absorbers in solar cells, and emitters in quantum technology. While exploring the chemistry and self-assembly of lead halide perovskite nanocrystals, a curious dichotomy of their reactivity has emerged. On the one hand, the ease of chemical transformations of lead halide perovskites is a powerful tool to tune their optoelectronic properties. On the other hand, the same reactivity is a cause of headache for researchers due to the sample instability under experimental conditions. In this contribution, I will discuss the dichotomy through examples of three transformations. The Good one converts bland Cs₄PbBr₆ into luminescent CsPbBr₃ nanocrystals and opens the way for Cs₄PbBr₆-CsPbBr₃ and CsPbBr₃@SiO₂ heterostructures.[1,2] The Bad one expels iodide from mixed halide CsPb(I:Br)₃ nanocrystals under illumination, impeding tuning of photoluminescence.[3] Lastly, the Ugly one morphs nanocrystals together, complicating an already non-trivial photophysics of ordered assemblies of CsPbBr₃ nanocubes.[4]

References

- [1] D. Baranov et al., Chem. Sci. **11**, 3986 (2020)
- [2] C. Rossi et al., Chem. Mater. **34**, 405 (2022)
- [3] M. Brennan et al., ACS Energy Lett. **5**, 1465 (2020)
- [4] D. Baranov et al., ACS Nano **15**, 650 (2021)

Controlling the metal/semiconductor interface in 2D-dimensional based devices

Andres Castellanos-Gomez¹

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The properties of electronic devices based on 2D materials are, in most cases, ruled to a great extent by the metal-semiconductor interfaces. In fact, the contact between the metals, employed for the electrodes, and the semiconductor 2D material typically lead to the appearance of Schottky barriers that have a strong effect on the electronic and optoelectronic properties of the fabricated devices. Controlling these interfaces, by proper selection of metal electrodes and appropriate electrode contacting techniques can be as important as selecting a good 2D semiconducting material. In this talk we will discuss the possibility of making “soft-van der Waals contacts” and how they can help to control the metal-semiconductor interface.

References

- [1] InSe Schottky Diodes Based on Van Der Waals Contacts. Qinghua Zhao, Wanqi Jie, Tao Wang, Andres Castellanos-Gomez, Riccardo Frisenda. *Advanced Functional Materials* (2020). DOI:10.1002/adfm.202001307S.
- [2] Approaching the Schottky–Mott limit in van der Waals metal–semiconductor junctions. Yuan Liu, et al. *Nature* 557, 696–700 (2018)

Semiconductor Nanocrystal Optoelectronics: from Advanced Heterostructures to Oriented Self-Assemblies of Colloidal Quantum Wells

Hilmi Volkan Demir^{1, 2}

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In this talk, we will introduce the emerging field of semiconductor nanocrystal optoelectronics, with most recent examples of their photonic structures and optoelectronic devices employing atomically-flat, tightly-confined, quasi-2-dimensional colloidal quantum wells (CQWs), also popularly nick-named ‘nanoplatelets’. Among various extraordinary features of theirs, we will show that these CQWs enable record high optical gain coefficients [1] and can achieve gain thresholds at the level of sub-single exciton population per CQW on the average [2], empowered by carefully engineering their heterostructures [3,4]. Next, we will present a powerful, large-area self-assembly technique for orienting these nanoplatelets (either all face-down or all edge-up) [5], which provides us with a tool to help engineering their interfaces. Using three-dimensional constructs of all-face-down self-assemblies of CQWs with monolayer precision, we will demonstrate ultrathin optical gain media and lasers of these oriented-CQW slabs [6]. Finally, we will show record high-efficiency colloidal LEDs using CQWs employed as the electrically-driven active emitter layer [7] and record low-threshold solution lasers using the same CQWs employed as the optically-pumped fluidic gain medium [8]. Given their current accelerating progress, these solution-processed quantum well materials hold great promise to challenge their epitaxial thin-film counterparts in semiconductor optoelectronics in the near future.

References

- [1] B. Guzelturk et al., HVD, *Nano Letters* **19**, 277 (2019)
- [2] N. Taghipour et al., HVD, *Nature Comm* **11**, 3305 (2020)
- [3] Y. Altintas et al., HVD, *ACS Nano* **13**, 10662 (2019)
- [4] F. Shabani et al., HVD, *Small* (2022) (*in press*)
- [5] O. Erdem et al., HVD, *Nano Letters* **19**, 4297 (2019)
- [6] O. Erdem et al., HVD, *Nano Letters* **20**, 6459 (2020)
- [7] B. Liu et al., HVD, *Advanced Materials* **32**, 1905824 (2020)
- [8] J. Maskoun et al., HVD, *Advanced Materials* **33**, 2007131 (2021)

Cathodoluminescence Spectroscopy of Silicon nanoparticles

Saskia Fiedler^{1,2}, P. Elli Stamatopoulou¹, A. Assadillayev³, Christian Wolff¹, Hiroshi Sugimoto⁴, Minoru Fujii⁴, N. Asger Mortensen^{1,5}, Søren Raza³ and Christos Tserkezis¹

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The fabrication of nanostructures with ever-decreasing sizes has increased the demand of suitable characterization methods which allow to determine their shape and size at the true nanoscale, and similarly important, enable the investigation of their optical properties beyond the diffraction limit. Due to its high spectral and spatial resolution down to the (sub-) nanometer range, electron beam-based techniques, namely cathodoluminescence (CL) has become a powerful characterization tool, particularly to study plasmonic and dielectric nanostructures. However, the interpretation of the resulting spectral CL maps is not always unambiguously straightforward.

In this work, Mie resonances in single Si nanospheres of different sizes have been systematically studied, using experimental CL spectroscopy and an analytical CL model. For smaller spheres ($r \sim 75$ nm), the eigenmodes can be unequivocally identified, with relative changes in intensity of the electric and magnetic dipole depending on the electron beam position within the sphere. However, in larger spheres ($r \sim 105$ nm), the modal assignment becomes increasingly difficult due to a larger number of Mie modes in the visible spectral range. Additionally, penetrating electron beams generate two radiating dipoles at the two Si interfaces – due to the electron and its image charge collapsing at those interfaces – which can, depending on the electron beam's velocity and its path length inside the particle, produce distinct resonances or dips (constructive or destructive interference of those two radiative dipoles). It is demonstrated that superimposed on the eigenmodes of the studied nanospheres, these resonances can distort the recorded spectrum and lead to potentially erroneous assignment of modal characters to the spectral features. An intuitive analogy is developed to unambiguously distinguish those resonance induced by transition radiation from the nanoparticle-specific Mie resonances.

High Quantum Yield, Broadband, and Delayed Emission in Two-dimensional Tin Iodide Perovskite Nanosheets

S. Ghimire,¹ R. Lesyuk,¹ and C. Klinke^{1,2,3}

¹ *Institute of Physics, University of Rostock, Rostock, Germany*

² *Center for Interdisciplinary Electron Microscopy (ELMI-MV), Department “Life, Light & Matter”, University of Rostock, Rostock, Germany*

³ *Department of Chemistry, Swansea University, Swansea, United Kingdom*

In recent years, two-dimensional (2D) halide perovskites have shown promising results in solar energy harvesting, lighting, photodetection, and photocatalysis [1]. While lead-based perovskites are toxic, tin halide perovskites suffer from poor quantum yield and intrinsic instability due to the oxidation of Sn²⁺. Therefore, the demand for stable and highly luminescent lead-free 2D halide perovskites is increasing. Here, we report an improvement in the photoluminescence quantum yield from <1% in parent 2D octylammonium tin iodide perovskite nanosheets to ~25% in their structural variant. Solvent and light induce a structural transformation in these perovskite nanosheets at room temperature and shifts the bandgap from the visible to the UV region, resulting in broadband and delayed emission with a large Stokes shift. We discuss the observed optical properties in terms of self-trapped excitons localized in the tin iodide clusters and octahedral distortion present in the nanosheets [2]. Such a broad and intense self-trapped excitonic emission is promising for white LEDs.

References

- [1] S. Ghimire, K. Oldenburg, S. Bartling, R. Lesyuk, C. Klinke, *ACS Energy Lett.* **7**, 975 (2022)
- [2] S. Ghimire, C. Klinke, *Nanoscale* **13**, 12394 (2021)

Electronic structure of InAs quantum dot solids: influence of dimensionality and stoichiometry

R. V. H. Hahn¹, E. S. Skibinsky-Gitlin¹, S. Rodríguez-Bolívar¹, M. Califano², and F. M. Gómez-Campos¹

¹Dpto. Electrónica y Tecnología de los Computadores, Univ. de Granada, Spain

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Periodic quantum dot solids are new materials in which quantum dots are periodically distributed in space [1]. The properties of these materials are explored to find applications in new photovoltaic devices. In order to shed light on these future applications, investigating carrier transport [2] and light absorption are of paramount importance [3]. We present the electronic structure of one- (1D), two- (2D) and three-dimensional (3D) quantum dot solids made of 12 Å radius InAs quantum dots. Two different stoichiometries are studied. Configuration A has an arsenic-rich surface while in configuration B the surface is rich in indium. Figure 1 shows the electronic configuration in the studied configurations. The interdot distance is one-bond length. All the arrays show flat miniband structure in the valence band regardless dimensionality and stoichiometry due to the weak coupling of the valence band wavefunctions in InAs between neighbouring dots because of the greater hole effective masses. About the minibands in the conduction band, configuration A shows wider minibands than configuration B due to a greater interdot coupling in the former which can be attributed to the atomic distribution in the interdot facets. About dimensionality, three-dimensional configurations exhibit greater miniband curvatures because of greater coupling with neighbours (6 neighbours vs 4 and 2 in two- and one-dimensional arrays respectively). This will influence the effective mass for carrier transport in these quantum dot solids.

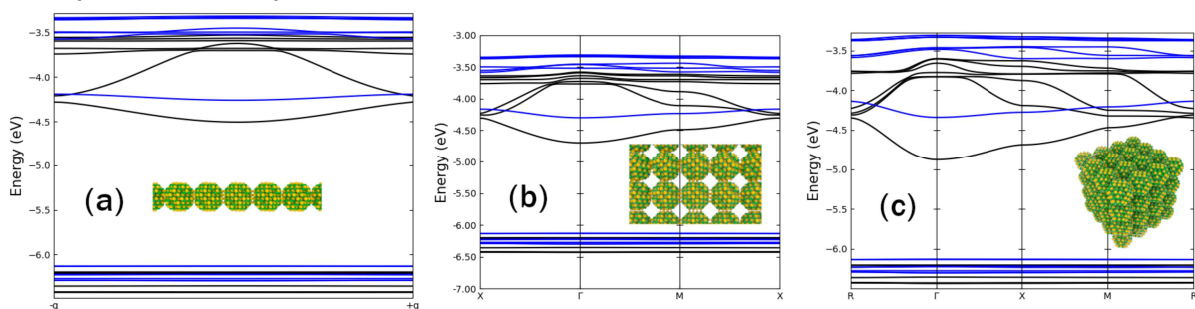


Figure 1: (a) one-, (b) two- and (c) three-dimensional quantum dot array electronic structures. Black (blue) lines are for configuration A (B). Yellow and green spheres represent arsenic and indium atoms respectively in configuration A. Configuration B has the inverted stoichiometry.

References

- [1] T. Hanrath, J. Vac. Sci. Technol. A, **30**, 030802, (2012).
- [2] N. P. Brawand et al., Chem. Matter., **29**, 1255-1262, (2017).
- [3] A. A. Chistyakov et al., J. Phys. Chem. Lett., **8**, 4129-4139, (2017).

Femtosecond electronics across nanostructured interfaces

A. Holleitner

Walter Schottky Institute and Physics Department, TUM, Germany

Recent work on ultrafast on-chip electronics explores electromagnetic phenomena at the frontier between electronics and optics in the frequency range between 100 GHz and 10 THz [1]. Recent examples include the exploration of the quantum critical optical conductivity of graphene [2] as well as the ultrafast transport of hot electrons within two-dimensional materials [3-6] and plasmonic circuits [7,8]. Interfaces in nanostructures play a crucial role in such electronic circuits, particularly for harvesting charge and energy transfer processes in organic [9] and inorganic [10] nanostructures which occur on ultrafast time-scales.

In the talk, I will introduce the occurring optoelectronic processes at nanostructured interfaces, and how to explore them utilizing ultrafast on-chip electronic schemes.

References

- [1] P. Zimmermann, et al. *Appl. Phys. Lett.* **116**, 073501 (2020).
- [2] P. Gallagher, et al. *Science* **364**, 158 (2019).
- [3] L. Prechtel, et al. *Nat Com.* **3**, 646 (2012).
- [4] N. Hunter, et al. *Nano Lett.* **15**, 1591 (2015).
- [5] E. Parzinger, et al. *Npj 2D Mater Appl* **1**, 40 (2017).
- [6] J.W. McIver, et al. *Nat. Phys.* **16**, 38 (2020).
- [7] C. Karnetzky, et al. *Nat Com.* **9**, 2471 (2018).
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Colloidal Quantum Nanowires: Structural, Optical, and Electronic Properties

Tobias Kipp

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In this lecture, a comprehensive overview over the structural, optical, and electronic properties of colloidal quantum nanowires (QNWs) will be given. These QNWs are quasi-one-dimensional II-VI semiconductor nanostructures, wet-chemically synthesized by the so-called solution-liquid-solid method. They exhibit diameters below about 15 nm and lengths up to several micrometers. Their optoelectronic properties strongly depend on the morphology, diameter, segmented crystal structure, surface modifications, and interfaces to conducting leads. For the investigation, we used a variety of different experimental techniques, like confocal time-, energy-, and space-resolved photoluminescence (PL) spectroscopy, transmission electron microscopy (TEM), atomic and electrostatic force microscopy (AFM and EFM), electrical transport measurements, scanning photocurrent microscopy (SPCM), X-ray diffraction (XRD), X-ray beam induced current (XBIC) and X-ray excited optical luminescence (XEOL) measurements.

We established a routine to determine the fraction of wurtzite and zincblende segments along CdS, CdSe, and CdTe QNWs by XRD measurements and modelling [1]. A detailed relationship between radial confinement and optical properties in CdSe QNWs could be established [2]. The diffusion of photo-generated charge carriers or excitons in axial direction was shown [3] and charge-carrier separation in bandgap engineered QNWs with heterostructured interfaces was proven [4]. By actively charging isolated CdSe QNWs with a biased AFM tip, the PL emission can either be enhanced or reversibly or irreversibly quenched [5]. Low-temperature PL investigations on individual QNWs revealed fundamentally new features that are hidden at room temperature. A multitude of sharp excitonic emission peaks arranged in two different emission bands is observed, which exhibit a complex blinking behavior, each on a different time scale, as well as different phonon couplings [6]. We showed how QNWs can act as the active element in fast and sensitive photodetector devices, exploiting the possibility to catalytically grow QNWs directly from conducting electrodes [7]. We investigate the axial conduction- and valence-band bending and electrostatic potential drop in contacted and biased QNWs by SPCM and scanning-force microscopy. The spatial resolution of these measurements can even be enhanced by scanning X-ray techniques, like XBIC.

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Colloidal 2D PbSe nanoplatelets with efficient emission reaching the Telecom O-, E- and S-band

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2D lead chalcogenide nanoplatelets and nanosheets are highly topical materials for near-infrared (NIR) optoelectronic applications, providing solutions with bandgaps tailored to the telecom O-, E- and S-Band.¹ While lead chalcogenide nanocrystals and thicker nanosheets are already extensively researched and well established, atomically thin nanoplatelets only recently moved into focus.²⁻⁴ Lead chalcogenide nanoplatelets combine the inherent advantages of 2D materials, such as monodispersity in thickness and increased exciton binding energies, with a large exciton-Bohr radius and the possibility of multiple exciton generation.⁵

In this work, we present 2D PbSe NPLs with cubic rock salt crystal structure synthesized at low reaction temperatures of 0 °C and room temperature.² The optoelectronic properties have been analysed using steady state and ultrafast transient optical spectroscopy. A lateral size tuning of the PbSe NPLs by adding small amounts of octylamine to the reaction and by controlling the temperature leads to excitonic absorption features in the range of 800 – 1000 nm (1.6 – 1.3 eV) and narrow photoluminescence (PL) seamlessly covering the broadband infrared spectral window of 900 – 1450 nm (1.4 – 0.9 eV). The PL quantum yield of the as-synthesized PbSe NPLs is more than doubled by a postsynthetic treatment with CdCl₂ (e.g. from 14.7 % to 37.4 % for NPLs emitting at 980 nm). The origin of this increase being the decreased contribution of trap-state emission is revealed PL lifetime measurements and transient absorption measurements. Our results open up new pathways for a direct synthesis and straightforward incorporation of colloidal PbSe NPLs as efficient infrared emitters at technologically relevant telecommunication wavelength.

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A Colloidal 2D Semiconductors Covering Visible to Telecom Window Wavelengths - Combining Chemistry and Spectroscopy for Innovative Optoelectronics and Photonic Quantum Technologies

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Colloidal 2D semiconductors (nanosheets (NSs) and nanoplatelets (NPLs)) are only a few atom layers thick and strongly quantum-confined in their thickness dimension. This leads to increased exciton binding energies in the structures and optical properties that are wet-chemically tunable from visible to infrared wavelengths. Synthetic fine-tuning of the NSs and NPLs to control their narrow absorption and efficient emission is highly interesting for photonic and optoelectronic applications.[1] I will touch on recent results on the synthesis of colloidal 2D transition metal dichalcogenides (WS₂ and MoS₂). By adjusting the Mo- and W-precursor concentration and reaction times, a control on the formation of the semiconducting vs. the metallic TMDC crystal phase during the reaction is gained and followed by XPS. We applied micro-photoluminescence spectroscopy to study semiconducting WS₂ mono- and multilayer photoluminescence comparable to exfoliated WS₂ for the first time.[2]

The second part of my talk is dedicated to our results on the direct synthesis of infrared-emitting 2D PbSe NPLs. By synthetically tuning the lateral size of the NPLs, we obtain efficient emission of the NPLs covering the telecom O-, E- and S-band, respectively.[3,4] Infrared emitting NPLs are highly interesting for emerging photonic quantum technologies, e.g. single photon emission at technologically relevant wavelengths.

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Role of Mn–Mn coupling in photoluminescence kinetics of doped ZnS nanoplatelets

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Mn-doped ZnS colloidal nanoplatelets (NPLs) present an attractive heavy-metal-free platform to study the optical properties of doped nanocrystals^{1,2}. Due to the ultrathin shape, the band structure and hybridization of Mn and ZnS orbitals are strongly influenced by quantum confinement and dopant location leading to a different decay kinetics of photoluminescence (PL) in comparison with the bulk. Additionally, tunable degrees of coupling between the dopants contribute to the complexity of relaxation pathways. Here, the location- and concentration-dependent time-resolved (TR) PL signatures of ZnS:Mn NPLs are shown both by experiments and with the help of density functional theory (DFT) calculations. The effect of the surface was deciphered by the post-synthetic shell overgrowth by c-ALD. The origins of the slow, intermediate and short decays have been assigned to corresponding transitions (*p-d- or s-p-character*) of isolated, weakly coupled, and strongly coupled Mn²⁺ ions. The model offers a potential possibility to form localized states with predicted lifetimes and emission wavelengths based on location-dependent and Mn–Mn distance-dependent effects on PL in zinc sulfide NPLs. It can also be used as a tool for the assessment of the doping level, homogeneity and surface contribution to the PL of Mn-doped nanosystems.

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By design light matter interaction in nanocrystal array, a step toward active nanophotonics

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One key issue raised by the use of nanocrystals for photoconduction is the discrepancy between the absorption depth (few μm) and the charge diffusion length (<100 nm). In other words, thick samples are desirable to absorb photons, but photocarrier collection remains limited. To face this challenge the incident light has to be « focused » on a thin slab of semiconductor whose thickness is compatible with transport. There comes the need to reshape the incident light propagation which can be obtained through the introduction of light resonators such as plasmonic gratings and Fabry-Pérot cavities. Here, I will review some of the recent developments of the group toward this direction.

To start, I will discuss the introduction of guided mode resonators. With this strategy the incident plane wave is transformed into a mode propagating along the substrate thus enabling several passes of the light through the film which enhanced absorption. We have applied this strategy to several narrow band gap nanocrystals [1], to sensitize perovskite in the infrared [2] and more recently to intraband absorbing devices [3]. I will also show that this strategy can be easily implemented in various device geometries such as planar photoconductors and phototransistors [4] or in vertical photodiodes [5]. Beyond quantum confinement, the design of the light-matter coupling enables a new degree of freedom to tune the spectral response of a device through the geometrical factor of the device. Finally, I will discuss how light management strategies can be used to design active devices, whose spectral response can be reconfigured via a bias application [6].

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Interface design across the scales in molecular and hybrid solids

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Interfaces and interphases are ubiquitous in mono- and multicomponent materials and may even dominate their properties. This is especially true for nanomaterials in which surfaces and interfaces can serve as a design principle to control the chemical, optoelectronic, or transport properties of a nanoscale architecture.

In layered molecular solids such as covalent organic frameworks (COFs), insights into the nature and functional role of interfaces in charge transport and energy conversion is scarce, due to a lack of local probes that are sensitive to the in- or out-of-plane structure of the interfaces. And yet, the structure of (in-plane) grain boundaries,¹ (out-of-plane) stacking of the layers,² and inclusion of functional units (e.g. catalysts) into the pores of COFs^{3,4} – each corresponding to or generating different types of interfaces – can have a profound influence on the (opto)electronic and catalytic properties of these molecular materials.

In this presentation, I will discuss the design, analysis and utilization of homo- and heterointerfaces in molecular materials and “artificial solids” made from combinations of 2D materials by “molecular beaker epitaxy”.⁵ Examples will be given that highlight the different types of homo-, hetero- and dynamic interfaces that can be sculptured from the atomic to the nanoscale to serve various purposes in photocatalysis, molecular sensing,⁶ and beyond.

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Optoelectronic Processes in Low Dimensional Systems

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By integrating bottom-up synthesis with top-down lithographic techniques, various single-crystalline nanowires have been synthesized. They are characterized by different methods such as electron microscopy, photoluminescence, photoconductance, and electrical transport measurement. Using ZnO nanowires as an example, they are configured as field effect transistors (FET) and have demonstrated a range of potential applications as UV emitters and photodetectors. In order to optimize the device performance, surface passivation procedures are conducted and the nanowire FETs exhibit orders of magnitude improvement in the on/off ratio, field effect mobility and sub-threshold swing.

On the other hand, we will describe the recent research progress on Weyl semimetals. One of their most intriguing optoelectronic properties is their polarization dependent photocurrent response, enabled through a nonlinear process [1,2], which can open up new opportunities for optical polarization detection. We have characterized the polarization dependent photocurrent response on prototypical TaAs with a confocal imaging system.

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Gaining insights into the ABX₃ chalcogenide material BaTiS₃ for NIR applications

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Near infra-red optoelectronic materials are of special interest because of their demand in spectroscopic and telecommunication devices. To date, the frequently used materials consist of compounds containing indium, gallium, germanium, arsenic, and/or lead, which is also a banned substance for commercial use in the EU. Therefore, the urge to use a new low band gap material with more earth-abundant, stable, and low-toxicity elements leads to the class of ABX₃ chalcogenides. In this class of materials, BaTiS₃ with a small band gap of around 0.5eV (2500nm) is one promising material meeting the requirements. Recent colloidal synthetic attempts were successful in creating the material in either nanorod or nanoparticle formfactors with the lowest energy absorption feature in the NIR region. To gain deeper insights in the formation of this interesting material and to understand more about the formation of ABX₃ chalcogenides in general, intermediate growth products are extracted and analyzed to track the synthetic route. The optical properties collected from UV-VIS absorption measurements and transient absorption spectroscopy (TA) will be presented. Additionally, ligand exchange and processing conditions for device fabrication is discussed.

Spectroelectrochemistry of CdSe Quantum Dots

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Semiconductor quantum dots (QDs) have size tunable emission. However, their luminescence is punctuated by blinking, i.e. random on-off events and spectral diffusion. This is partly due to ionization of the nanocrystal which leads to formation of trions – negatively or positively charged particles. These trions emit weakly due to Auger recombination and recombination through surface states. While spectroelectrochemical studies of films of QDs have been carried out, there are few such studies of QDs in solution.

We present results on the systematic injection of electrons and holes into solvated CdSe quantum dots and nanoplatelets (using electrochemical methods) to create trions. Spectroelectrochemistry provides a way to monitor the spectra of QDs as a function of applied potential. We provide spectra of trions as a function of the charge and establish the energy levels for injection of charges. We show that electron injection is reversible and that the negative trion is long-lived (see Figure 1).

Under a high cathodic bias, injection becomes diffusion limited and the number of electrons being injected can be calculated from the Cottrell equation. We discuss the differences between injection into nanoplatelets and quantum dots and the role of wide-bandgap, shell layers on the injection process. Nanoplatelets (NPLs) show quite different properties and exhibit potential induced photobrightening. We explain this effect and contrast the two systems (QDs and NPLs).

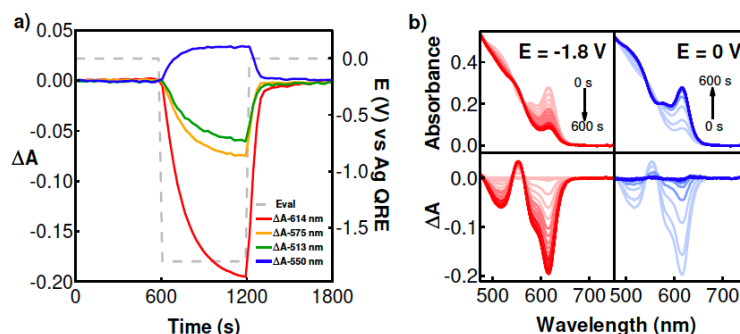


Figure 1: Spectroelectrochemistry of CdSe quantum dots in THF. (a) Bleach signal vs time at different wavelengths following square pulse potential steps; (b) spectral changes due to exciton bleaching during cathodic and anodic steps.

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Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment

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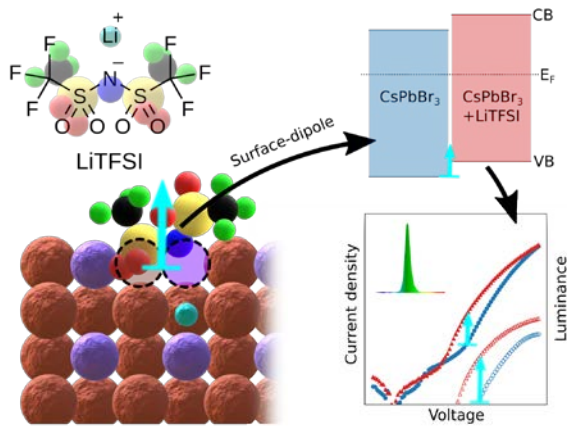
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Surface-defect passivation is key to achieving high photoluminescence quantum yield in lead halide perovskite nanocrystals.

However, in perovskite light-emitting diodes these surface ligands also have to enable balanced charge injection into the nanocrystals to yield high efficiency and operational lifetime. In this respect, alkaline halides have been reported to

passivate surface trap states and increase the overall stability of perovskite light emitters.

On the one side, the incorporation of alkaline ions into the lead halide perovskite crystal structure is considered to counterbalance cation vacancies, while on the other side, the excess halides are believed to stabilise the colloids.

Here, we report an organic lithium salt, viz. LiTFSI, as a halide-free surface passivation on perovskite nanocrystals. We show that the treatment LiTFSI has multiple beneficial effects on lead halide perovskite nanocrystals and LEDs derived from them. We obtain higher photoluminescence quantum yield and longer exciton lifetime, and a radiation pattern that is more favourable for light outcoupling.

The ligand-induced dipoles on the nanocrystal surface shift their energy levels toward lower hole-injection barrier.

Overall, these effects add up to a four- to seven-fold boost of the external quantum efficiency in proof-of-concept LED structures, depending on the colour of the used lead halide perovskite nanocrystal emitters.

In-plane anisotropic properties of two-dimensional MoO₃

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Molybdenum trioxide (MoO₃) in-plane anisotropy has increasingly attracted the attention of the scientific community in the last few years [1, 2]. Many of the observed in-plane anisotropic properties stem from the anisotropic refractive index and elastic constants of the material [3,4] but a comprehensive analysis of these fundamental properties is still lacking. Here we employ Raman and micro-reflectance measurements, using polarized light, to determine the angular dependence of the refractive index of thin MoO₃ flakes. We study the directional dependence of the MoO₃ Young's modulus using the buckling metrology method, finding large in-plane anisotropic mechanical properties [5]. Raman shift rates also exhibit distinctive anisotropic strain responses with an intriguing positive shift in wavenumber in polarized Raman micro-reflectance measurements, opposite in sign to almost the rest of the reported materials.

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Modelling Mechanical Properties of Gold Nanoparticle Arrays with Molecular Dynamics

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Cross-linked gold nanoparticle arrays are of great interest due to their various applications such as sensors (e.g., strain sensors, chemiresistors). In the last decades, huge emphasis was put on tuning the sensor responses, for example, by changing the length of the linker, or by using different ligand mixtures (e.g., monothiols/dithiols)[1]. Still, experimental methods to analyse those arrays usually can not provide structural insights on an atomistic level. An accurate model of the structure is, however, crucial to obtain a deeper mechanistic understanding of the mechanical and charge transport properties, especially in mixed ligand systems and in the presence of analyte molecules. We started by creating a simple model of two dithiol-cross-linked gold surfaces and investigated the influence of the length of the ligand, the addition of analyte molecules, and the replacement of dithiol molecules by monothiols on the surface-to-surface distance. The expected linear dependence of the distance from the alkane chain length can be observed, and the increase per CH₂ unit is comparable to experimental data[2]. An increase in the equilibrium distance when adding analyte molecules (such as pentane) can be observed, which resembles the swelling that is expected to be the prominent contribution to the functionality of this type of chemiresistors. In future work, we want to study how these factors (analyte molecules, mixtures of monothiol and dithiols) influence the charge transport between the two surfaces and give insights into possible charge transport pathways.

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Observing Quantum-Confinement Effects on the In-Plane Translational Motion of Excitons in CdSe Nanoplatelets

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Colloidal CdSe nanoplatelets (NPLs) can be made with a thickness of atomic precision in the range of about one to a few nanometers only. The lateral sizes are of the order of several to tens of nanometers. The thickness is less than the bulk exciton bohr radius and consequently leads to strong effects of spatial confinement on the internal energy of an exciton. Variation of the thickness of a NPL thus allows one to tune the photoluminescence (PL) and optical absorption spectra.

Interestingly, however, the experimental shape of PL and absorption spectra also depends on the lateral sizes of a NPL. To date, the latter has not received much attention, with the exception of a few (mainly theoretical) studies and the origin of this effect has been inconclusive.

We measured the PL and absorption spectra for a series of NPLs with different lateral sizes and find that the dependence of the optical spectra on the lateral size is fully explained by taking into account the quantum-confinement effects on the translational motion of excitons in the plane of the NPLs.[1] The spectra of all samples considered can be reproduced very accurately by a theoretical description of exciton energies and oscillator strengths based on the quantum mechanical particle-in-a-box model and the known size-distribution of the NPLs.

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Dynamic screening of quasiparticles in WS₂ monolayers

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In recent years, 2D materials attracted substantial scientific interest from a fundamental perspective, and for their potential technological applications. In this context, transient changes of the optical properties, in particular the A exciton resonance (AX) were investigated, which displays complex dynamics (linewidth broadening, blue, and red shifts) depending on substrate, excitation density, and photon energy. However, the particular interplay of the dielectric screening of the substrate and the dynamic screening of quasi-free carriers and excitons on exciton binding energy and free carrier band gap remains elusive.

We access the time-dependent dielectric function of the A exciton in monolayer WS₂ on different substrates using reflectivity and transmittivity contrast experiments and applying the 2D linearized [1] and the Fresnel transfer matrix model, tracking peak shift and broadening of the resonance upon photoexcitation [2]. These are then described by a simple two/three-level model based on the time evolution of the photo-excited carrier and exciton populations. We determine exciton formation and recombination times, the Auger recombination rate, broadening parameters of quasiparticle scattering events, and the renormalization parameter the free carrier band gap in good agreement with literature values where available. This allows the disentanglement of the thermal, exciton, and free carrier contribution to the XA peak shift and broadening as well as to conclude that (i) linewidth broadening is dominated by exciton scattering, (ii) exciton screening acts mainly on the exciton binding energy, while (iii) quasi-free carriers are largely responsible for band gap renormalization. These findings constitute a comprehensive picture of the non-equilibrium dynamics in monolayer WS₂ and will pave the path towards the application and control also of other 2D materials' transient properties.

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Topological Wannier Excitons in Bismuth Chalcogenides Nanosheets

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We analyze the topology and dispersion of bulk Wannier excitons in nanosheets of topological insulators in the family of bismuth chalcogenides. Our main finding is that excitons also inherit the topology of the electronic bands, quantified by the skyrmion winding numbers of the constituent electron and hole pseudospins as a function of the total exciton momentum. We furthermore show that every s-wave exciton state consists of a quartet with a degenerate and quadratically dispersing nonchiral doublet, and a chiral doublet with one linearly dispersing mode as in the transition metal dichalcogenides. We also consider the topological edge states of the chiral excitons.

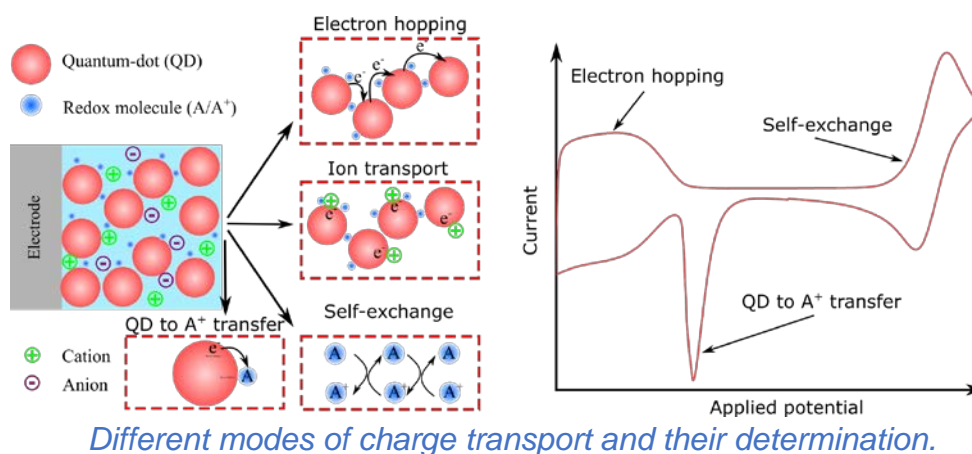
Charge percolation in QD–molecule assemblies

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Quantum dots (QDs) show great promise in next-generation applications, which often require linked redox moieties to function, such in solar cells, electrocatalysts and chemical sensors. Control over charge transport across these QD–molecule assemblies is crucial for their implementation in next-generation semiconductor devices. A problem however is that the mechanisms of charge transport are still little understood.

We found that charge transfer across QD–molecule assemblies can occur via electron transfer between QDs (electron hopping) and between redox molecules (self-exchange), while molecular acceptors act as electron sinks inducing transfer from QDs. All these processes are accompanied by counterion transport to keep electroneutrality. This complexity of mechanisms can be individually controlled and studied by electrochemically modulating the Fermi level. Self-exchange is turned on at the formal potential of the redox couple, while electron hopping through QDs and transfer from QDs to molecular acceptors is operative within the conduction band energy.



This study offers a path to understanding and engineering charge transport in QD–molecule assemblies that has been previously unexplored. It provides a platform that is of practical and fundamental importance. For example, it is ideal to put to test theories of electron transfer: self-exchange can be described using percolation theory, which usually assumes close contact, but this should be also influenced by long-range electron transfer, a theoretical prediction that still needs to be experimentally tested. Practically, conduction paths through self-exchange could be either beneficial or detrimental depending on the application and understanding how to control this process could enable improved device efficiencies and the development of new applications.

Tailored Interfaces with and Defects in Single-Walled Carbon Nanotubes

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The specific interaction and selective wrapping of certain single-walled carbon nanotubes (SWNTs) with conjugated polymers has enabled the sorting and purification of large amounts of semiconducting and even monochiral SWNTs that can be applied in a wide range of (opto-)electronic devices with outstanding charge transport properties [1]. Furthermore, their near-infrared emission properties are tunable by intentional doping [2, 3] and by the controlled introduction of different luminescent sp^3 -defects [4]. These quantum defects with characteristically red-shifted emission and long photoluminescence (PL) lifetimes enable higher PL quantum yields and single-photon emission at room temperature. They can be created in a controlled manner in polymer-wrapped semiconducting nanotubes in organic solvents using diazonium chemistry with a phase-transfer agent [5]. Various substituents are possible including the stable and neutral perchlorotriphenylmethyl (PTM) radical, which directly interacts with the sp^3 -defects [6]. Furthermore, the type of defect emission (E_{11}^* or E_{11}^{*-}) is governed by the precise binding configuration for chiral (6,5) SWNTs. A simple synthetic protocol relying on nucleophilic addition instead of radical-based reactions facilitates the introduction of only the more red-shifted E_{11}^{*-} defects with even longer PL lifetime and high single-photon purity [7].

Here, I will give an overview of our recent progress on the targeted functionalization of polymer-wrapped (6,5) SWNTs, their emission and charge transport properties with and without defects [8] and their application in devices.

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Abstracts of Posters

(in alphabetical order)

Coupled Organic-Inorganic Nanostructures photodiodes using single and heterostructure types of ligands

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The influence of the ligands in coupled organic-inorganic nanostructures (COINs) on the performance of optoelectronic devices is investigated. We fabricate photodiodes based on pentacene and PbS nanocrystals coupled to organic ligands like 1,2-ethanedithiol (EDT) and tetrabutylammonium iodide (TBAI) and a combination of both, EDT and TBAI, as a heterostructure. These ligands were first separately used to fabricate a single ligand-type of organic-inorganic device and later compared with a heterostructure of PbS-EDT and PbS-TBAI. To tune the optical energy gap of COINs to align with the triplet level of pentacene T1, it was necessary to choose the suitable particle size. For this purpose, ultraviolet photo-emission spectroscopy (UPS) was used to determine the energy of the highest occupied molecular orbital (HOMO) and the work function of COINs, while the energy of the lowest unoccupied molecular orbital (LUMO) of COINs was estimated subsequently by adding the exciton binding energy and the optical band gap to the measured HOMO energy. Devices with heterostructure COINs achieve a higher short circuit current than COINs with single type of the ligands. Finally, even if the requirements of proper energy level alignment are satisfied, the photodiodes' performance was affected by the morphology of COINs. This finding has been demonstrated by atomic force microscopy (AFM) and transmission electron microscopy (TEM). Incident photon to current efficiency (IPCE) shows different excitonic absorption peaks in the visible range for different stacks. Radiative recombination process is detected by measuring the electroluminescence (EL).

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Alloyed CdSe_xS_{1-x} nanoplatelets with continuously tunable blue-green emission

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Cadmium chalcogenide nanoplatelets represent a promising class of semiconductor nanomaterials for optoelectronic applications since they exhibit properties, which are superior to the properties of nanocrystals of other dimensionalities. One of the particular features of nanoplatelets is the ability to precisely control their thickness down to one atomic monolayer. Due to this, they are monodisperse in quantum confinement direction and as a result exhibit narrow absorption and emission lines free from inhomogeneous broadening. On the other hand, the possibility to control thickness only in discrete steps prevents the precise spectral tunability of nanoplatelets.

One of the potential solutions to this problem is the modification of nanocrystal composition through the synthesis of alloyed nanoparticles. Direct synthesis of such nanocrystals is complicated by the need to balance the reactivity of precursors, which can be achieved by modifying their composition, introducing additives into the reaction mixtures, changing the reaction temperature, etc. Most of these changes, however, are not applicable for the synthesis of nanoplatelets since they form only in a limited range of conditions, which are oftentimes incompatible with the conditions for precursor reactivity tuning.

In this work, we employ highly reactive sulfur and selenium sources for the synthesis of nanoplatelets, which allow straightforward and precise tuning of nanoplatelet composition and hence the position of their absorbance and photoluminescence bands. We also demonstrate that by changing the reaction temperature one can prepare nanoplatelets with different thicknesses, which further extends the spectral range of the synthesized nanocrystals. In addition, prepared nanoplatelets have a relatively small lateral size and well-defined shape, which reduces the number of surface defects in the nanocrystals, and as a consequence nanoparticles exhibit bright emissions with > 30 % quantum yields.

Exciton Energy funneling in Perovskite-TMDC (0D-2D) Hybrid System

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Van der Waal structures such as transition metal dichalcogenide (TMDC) are a class of layered semiconducting materials. They show an indirect to direct bandgap transition when peeled down to a monolayer. The monolayer of these materials with improved light-matter interaction, carrier mobility, strength makes them an excellent component in optoelectronic devices such as LEDs, photodetectors, phototransistors, etc. The atomically thin nature of these materials results in a weak (<1%) light absorption which is crucial for efficient optoelectronic devices. Integration of strong light absorbing, wider bandgap 0D materials such as CdSe, CdS, perovskite nanocrystals with TMDC monolayers can improve the carrier concentration in the monolayers due to exciton energy transfer between the two materials. New generation halide perovskites nanocrystals (NCs) such as CsPbBr₃ NCs with better stability, defect tolerance and bandgap tunability in particular are potentially the best suited candidate as the light sensitizing material. A heterostructure combination of the two systems (0D-2D) can show new electronic properties. A plethora of options available in these two classes of materials in terms of band offsets and bandgaps can lead to both type I and II systems.

In this contribution, we present a large exciton energy funneling in a 0D-2D heterostructure of new generation CsPbBr₃ (di-dodecyl, dimethyl ammonium as ligand) and MoSe₂ monolayer. MoSe₂ and CsPbBr₃ heterostructure form a type I structure with MoSe₂ being the lower bandgap material. We use steady-state and time-resolved μ -PL spectroscopy techniques to probe the photo-induced energy transfer between a set of different CsPbBr₃ NCs and MoSe₂. Spectroscopy results will be discussed in detail in terms of exciton energy transfer and its efficiency will be compared to literature.

OPTICAL, STRUCTURAL AND OPTOELECTRONIC PROPERTIES OF PULSED LASER DEPOSITION PBS THIN FILM

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Lead sulfide (PbS) nano-structured film has been grown on quartz substrates by the PLD technique. The deposited films were characterized by X-ray diffraction (XRD), selected area electron diffraction (SAED), transmission electron microscopy (TEM) and scanning electron microscopy (SEM). Formation of cubic phase of PbS nano crystals is proven. The absorption and emission spectra were measured for different thicknesses of the films. $I-V$ characteristics and photoconductivity of the deposited film were also measured. The results indicate an efficient performance of the deposited films as an optical detector.

The UV-PLD was performed with a XeCl excimer laser operating at 308 nm. PbS films were deposited on quartz substrates by ablating the pure PbS galena target (the common PbS mineral of cubic crystal structure). The target-to substrate distance was 5 cm. The substrate temperature and ambient pressure were kept at 350°C and 5×10^{-5} torr, respectively. The samples were deposited using a laser energy density of 2.5 J/cm² at a repetition rate of 100 Hz and ablation durations of 2.5 and 4 min. The film's thickness was measured by an optical interferometer. No post-deposition annealing was performed. The crystal structure of the deposited films was characterized by X-ray diffraction (XRD) using PRO pw 3040/60 (PANalytical) advanced X-ray diffractometer with CuK α ($\lambda = 1.54 \text{ \AA}$) radiation. The particle size and surface morphology was studied using transmission electron microscope (LIBRA 200 FE Zeiss) and scanning electron microscopy (FEI Quanta 3D 200i). The optical properties of the nanoparticles were measured using Perkin Elmer UV-Visible spectrophotometer. Also, the $I-V$ characteristic curve of the deposited film was measured at different values of temperatures and compared to that of the bulk target. The result of applying the prepared film as a sensor for the NIR radiations is also presented.

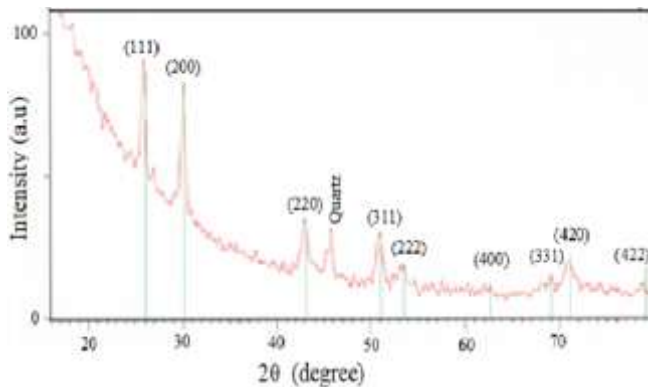


Fig. 1 XRD of PbS film grown on quartz substrate at T = 350°C

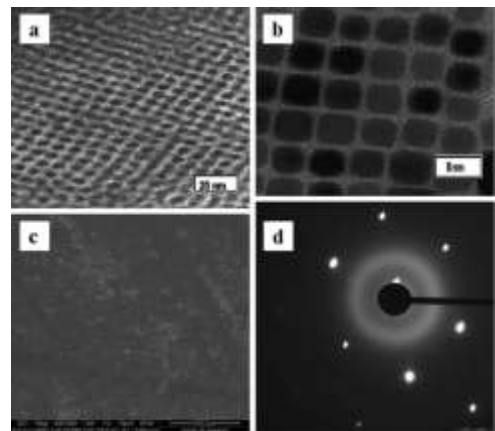


Fig. 2 (a) TEM image (scale bar 20 nm), (b) localized TEM image (scale bar 5 nm), (c) SEM image and (d) SAED pattern of PbS nanostructure deposited on quartz substrate

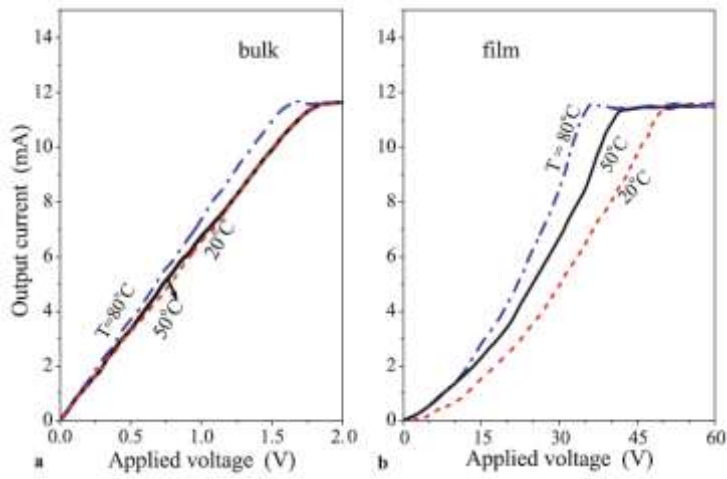


Fig. 3 I –V characteristic curves of PbS samples, in case of (a) bulk target and (b) deposited films, at temperatures values of 20°C, 50°C and 80°C

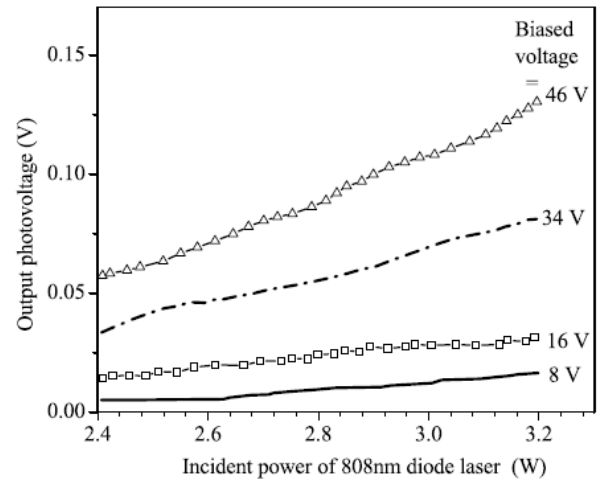


Fig. 4 Response of PbS films to incident laser powers of 808 nm at different applied bias voltages

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Thin Films via Deposition of Colloidal Nanocrystals for High Order Harmonic Generation

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Colloidal semiconductor nanocrystals like quantum dots (QD), nanorods, nanoplatelets etc. are of interest to a broad range of optical and electronic applications having electronic properties which are tunable by variations in size and shape and showing discrete energy levels due to spatial quantization of electron and hole motion instead of a band structure as in the bulk. Fabrication of optoelectronic devices; photovoltaic cells, photodetectors, LEDs using colloidal nanocrystal has been addressed in the last few years. Further, these structures are of highest interest in non-linear optical (NLO) applications. It was predicted theoretically that the efficiency of HHG in quantum confined structures is significantly enhanced in comparison to bulk solids due to a reduction of quantum diffusion as a result of the reduced density of the available states. To enable the investigation of the impact of quantum confinement on the HHG process we report on methods to generate thin films from colloidal QDs with various sizes entering different regimes from strong confinement ($r < \text{Bohr's radius}$) to weak confinement ($r > \text{Bohr's radius}$) and with tunable inter QD coupling via surface ligands with different lengths. To achieve such solid layers of QDs of certain thicknesses, spin coating and drop casting methods are used. Conventional steady-state spectroscopy (absorption, PL spectroscopy) along with time-resolved spectroscopy (e.g. transient absorption) delivers information on the degree of coupling between the quantum dots in the generated layers. Additionally, by applying Raman spectroscopy changes in the phonon confinement with QD size and modification of the surface ligands in QDs are monitored. First experimental results on HHG in these quantum dot layers demonstrate the dependence of harmonic spectra on size of the quantum dots reflecting the impact of size dependent electronic structure on the HHG process.

Surface Treatment of Colloidal 2D PbSe NPLs for Emission Enhancement at Telecom Wavelengths

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The direct synthesis of lead chalcogenide (PbX, X = S, Se, Te) based 2D semiconductors, so-called nanoplatelets (NPLs), yields photoluminescent materials with strong excitonic effects at room temperature ^[1] and high potential for optoelectronic applications at telecommunication wavelengths. ^[2]

We report a facile and direct wet chemical approach toward colloidal 2D PbSe NPLs with high emission efficiency. ^[2] The NPLs exhibit excitonic features in the range of 800 – 1000 nm and photoluminescence in the range of 900 - 1500 nm, with the respective positions being precisely tuneable by adjusting the NPLs lateral size via the reaction conditions. Postsynthetic surface treatment with metal and organic halide compounds results in increased photoluminescence quantum yields up to 50 % and strongly pronounced optical features, ascribed to a reduction of non-radiative recombination in the NPLs as well as a stabilization of the band-edge state, by saturation of undercoordinated surface sites.

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Controllable doping of semiconductor nanocrystals via cation exchange

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Copper doped semiconductor nanocrystals (NCs) have been used as luminescent material in a range of applications which include the emerging light and display technologies. The vivid range of applications come with challenges of synthesizing these doped NCs and understanding their unique photophysical properties. Along with their unique photophysical properties they also exhibit photoluminescence (PL) properties similar to copper chalcogenide based NCs wherein the PL recombination centres are attributed to Cu related defect states in both class of materials. Thus, the study of PL mechanism of this class of material provides further insight into the rather obscure PL mechanism of copper chalcogenide based NCs. As compared to direct method of synthesis a cation exchange method happens to be a feasible route of synthesizing these doped semiconductor NCs in which the extent of doping can be easily controlled by adjusting the composition of the host and guest cations.

Here we present the synthesis of differently sized CdSe/ ZnSe/ Cd_xZn_{1-x}Se NCs doped with Cu. Starting with binary Cu_{2-x}Se, Cd²⁺ is introduced into the crystal structure which leads to an almost complete exchange of Cu⁺ with Cd²⁺ leading to the formation of Cu doped CdSe. In a similar approach, exchange with Zn²⁺ and simultaneous exchange with Cd²⁺ and Zn²⁺ is carried out. This have led to QDs with PL tuneable from the visible to the NIR depending on the extent of doping and size of the as synthesized NCs. In a size range of 5 nm to 9 nm the PL is tuneable from 990 to 1120 nm in Cu doped CdSe. A variation of ratio of Cd²⁺ and Zn²⁺ in Cu doped Cd_xZn_{1-x}Se leading to varied composition of the NCs synthesized exhibits PL tuneability from 600 nm to 800 nm. The CE pathway helps in preserving the initial cubic crystal structure of Cu_{2-x}Se NCs in the final NCs synthesized.

Motorized Stage Allowing Improvements in Strain Engineering in 2D Materials

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Strain engineering in 2D materials has received extensive attention. Research in the field has already demonstrated piezoelectricity[1], bandgap tuning[2] and enhancement of thermoelectric figures of merit[3]. However, typical straining setups consist of manual micromanipulators[4] and have measurement limitations in long time and short strain intervals. The experimental results also suffer from accuracy because of these limitations. Therefore, we constructed a new setup with a motorized vertical translation stage and controlled it by PC. After calibration, the lowest strain value has been found as $\sim 10^{-6}$ %. Then, we have tested the setup by performing differential reflectance, photoluminescence, Raman spectroscopy, IV measurement and photoresponsivity on monolayer MoS₂ with several cycles. Gauge factors calculated in each measurement were found comparable with the previous results in literature. The setup can be a good candidate for straining experiments in a long time in order to discover their performance optically and electrically. Moreover, the measurements demonstrate lower strain interval and more repeatable cycles can lead to higher accuracy as well.

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Split-Gate Photodiode Based on Graphene/HgTe Heterostructure with a Few Nanosecond Photoresponse

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Nanocrystals are a promising building block for cost effective infrared optoelectronics. When it comes to light sensing, the vertical geometry diode is the most commonly used geometry since it enables zero bias operation and thus low dark current operation. However, the time response of devices based on vertical stacks is limited by the RC time constant of the stack. Thus, it will be of utmost interest to design planar diodes whose capacitance is lower, to be able to design fast responding sensor.

Here we demonstrate the design of a dual gated phototransistor [2,3]. Each gate is used to generate respectively a p and n area in a channel made of HgTe NCs [1]. The latter present a cut-off wavelength around 2.5 μm , corresponding to the extended short wave infrared range. To ease the formation of the *p-n* junction, we use graphene as drain and source electrodes, which offer two advantages: (i) the work function tunability of the electrode and (ii) being partly transparent to the gate induced electric field, thus enabling the change of the NC carrier density also on the top of the electrodes. A few nanosecond photoresponse is measured: it's the fastest value reported so far for an HgTe NC-based device [3].

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Depletion Layer Engineering in Core-Shell Metal Oxide Nanocrystals

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The optical and electronic properties of metal oxide nanocrystals (MO NCs) strongly depend on the surface depletion regions, derived from the presence of surface states. MO NCs exhibit a localized surface plasmon resonance (LSPR), offering tunable characteristics enabled by doping, or via electrochemical or photochemical charging. Dynamic control over the LSPR makes MO NCs promising for several optoelectronic and storage applications. [1] By manipulating the NC depletion width, it is possible to control the features of the NCs. The mechanism behind this phenomenon is very complex, and not yet fully understood. [2] In particular, it is possible to engineer the depletion region by varying several parameters, including the material under consideration, the size of the NCs, the presence of multiple core-shell systems, etc. To do this, it is possible to calculate the energy band and carrier density profiles for NCs with different features. In this work, a new framework has been introduced in order to predict the behavior and physics under the MO NCs photodoping process, revealing that the charging mechanism is based on the electronic rearrangement of the energy bands. Numerical simulations were experimentally supported by studying the case of a core-shell structure of ITO/In₂O₃ NCs, by tuning the thickness of the shell, as well as post-synthetically, both by photodoping and reversible chemical reactions. The engineering of the depletion layer and the consequent manipulation of the electronic structure allows to significantly increase the sensitivity of LSPR and to target specific properties in MO NCs. The fine-tuning of the NCs band structure has enabled an improvement in the charge storage capacity, which represents a step towards fully light-driven energy storage devices. [2]

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Low-toxicity and Sustainable Chalcogenide Materials for Photovoltaic Application

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Investigating novel chalcogenide nanomaterials to improve the sustainability and performance of optoelectronic devices is of key importance to drive future research and make commercialization possible. We seek to exploit the unique features of colloidal nanocrystals. Properties like solution-processability, the size-dependent band gap, or the adjustment of the energy levels by the choice of ligands – all while shifting from lead (Pb) and cadmium (Cd) containing materials to more sustainable tertiary chalcogenides of low toxicity. First work on the usage of CuInS₂ as an alternative for Pb- and Cd-containing tertiary chalcogenide quantum dots (QDs) in photovoltaic (PV) devices will be discussed. By changing the device structuring and processing of our materials, we work towards finding the limiting factors and developing strategies to overcome the challenges present in switching from well-understood PbS QDs and CdTe devices to those using CuInS₂. For example, enabling efficient ligand exchange and finding the ideal absorber layer thickness (balancing light absorption and charge transport) are important steps for the investigation and improvement of the device performance. We seek to use the gained knowledge to optimize our devices and enable further studies on sustainable light absorbing nanomaterials and their applications.

Synthesis and Characterization of Hybrid Semiconductor-Metal Nanostructures for Photocatalytical Applications

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Hybrid semiconductor-metal nanostructures are suitable for photocatalytic applications. The underlying processes are the photoexcitation of electron-hole pairs inside the semiconductor and the subsequent spatial separation of electrons and holes across the metal-semiconductor interface, before the charge carriers can contribute to the catalyzed chemical reaction.

In this work, we investigate the photocatalytic activity of colloidal semiconductor-metal nanostructures consisting of a rod-shaped semiconductor nanoparticle with a single metal nanoparticle tip on one side of the rod. The semiconductor nanoparticles themselves are heterostructures consisting of a spherical CdSe or ZnSe core that is embedded into a CdS rod-shaped shell. The CdSe/CdS and the ZnSe/CdS material systems differ in their conduction and valence band alignment (type-I and type-II), which should influence the charge separation process necessary for photocatalytic reactions. We used a hot-injection method^[1,2] to synthesize these dot-in-rod (DR) structures. To provide the DRs with a platinum or nickel tip, a reduction reaction was applied.^[3,4] We want to measure the photocatalytic activity of the hybrid nanostructures in a colloidal solution by monitoring the production of hydrogen upon illumination. We expect the ZnSe/CdS type-II system exhibits a stronger catalytic activity than the CdSe/CdS type-I structure. This would indicate a more effective charge-carrier separation in the type-II semiconductor as compared to the type-I system.

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Optimized Cation Exchange for Mercury Chalcogenide 2D Nanoplatelets

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II–VI two-dimensional (2D) nanoplatelets (NPLs) exhibit the narrowest optical features among nanocrystals (NCs). The direct synthesis enables the growth of NPLs with thicknesses from 2 ML to 5 MLs. The introduction of halides ligands enables to tackle these values and then to extend the optical properties in the red range for CdSe NPLs^[1]. The optical properties have been further extended to the NIR range through the synthesis of Hg-based NPLs obtained from cation exchange on Cd-based NPLs^[2]. We have optimized this procedure for which a solvent, surface chemistry, and reaction conditions are rationally considered. This procedure is applied to the growth of alloyed HgSe_{1-x}Te_x NPLs with various compositions. They present a bright photoluminescence for all compositions. We also unveil a crossover from n- to p-type behavior in HgSe_{1-x}Te_x NPLs while increasing the Te content.

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Light-driven energy storage solutions based on the coupling between metal oxide nanocrystals and 2D materials

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Novel energy storage solutions are necessary to meet the needs of self-powered electronic devices and complete in a fast and efficient way the global transition towards renewable energy. Photovoltaic energy is primarily limited by the intermittent nature of the solar source and suffers from stability issues, conversion losses, and limitations related to the size of the photovoltaic devices. An innovative path to overcome these problems is the combination of energy conversion and energy storage aspects into a unique system. Here, we report a hybrid nanostructure based on Metal Oxide Nanocrystals (MO NCs) and MoS₂ monolayers capable of light-driven charging, behaving like a photocapacitor. The main mechanism at the core of the anticipated device is the so-called photodoping process, i.e. the possibility to add permanently extra charges into the electronic structure of MO NCs in a completely contactless way. The photodoping process of MO NCs attracted a growing interest in recent years, with photo-charging dynamics reported both in liquid and solid state devices. The results we achieved with the photodoping of the ultra-thin heterostructure suggest direct storage of photons energy as extra positive and negative charges, separated by nanometric distances. The photo-generated holes are quenched at the semiconductor's surface and injected into the MoS₂ monolayer, while the photo-excited electrons accumulate in the ITO nanocrystal (with an estimated average of 75 stored charges per NC). The careful design and nanofabrication of similar heterostructures could open the path towards all-solid-state solutions for the direct storage of the solar energy and novel optoelectronic devices.

Towards tunnel gaps for nanoscale on-chip ultrafast photoemission currents

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We demonstrate that pre-structured metal plasmonic nanogaps can be shaped on-chip to below 10 nm by femtosecond laser ablation [1]. We explore the plasmonic properties and the nonlinear photocurrent characteristics of such formed tunnel junctions. The photocurrent can be tuned from multiphoton absorption toward the laser-induced strong-field tunneling regime in the nanogaps, and gives rise to a field emission of ballistic hot electrons propagating across the nanoscale junctions. We show that a unipolar current of hot electrons is achieved in the metal plasmonic nanogaps by designing the plasmonic enhancement factors in the junctions to be asymmetric, which allows ultrafast electronics on the nanometer scale. Additionally, we investigate helium ion microscope (HIM) patterned graphene nanogaps for nonlinear photocurrent dynamics. We particularly demonstrate that femtosecond optical pulses in the near-infrared (NIR) applied to such nanogaps can drive electronic circuits with a prospective bandwidth of up to 10 THz [2].

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Magneto Assisted Underwater Bubble Manipulation

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Unexpected nucleation, growth and deposition of air bubbles in underwater systems, particularly in aqueous channel surfaces, deteriorate the functionality and the performance of the system.¹ We introduce a magneto responsive, underwater bubble collection, merging, transportation and manipulation system applicable on water-solid interfaces. Low surface energy, chemically modified ferromagnetic iron (Fe) particles show underwater superaerophilicity together with magneto responsiveness. Therefore, underwater inserted these magnetic particles were magnetically guided and then attracted to the deposited air bubbles due to their superaerophilicity. Subsequently, by displacing the gradient magnetic field, the attracted air bubbles were transported and thus, easily removed from the underwater surface or microfluidic channel, Figure 1. This simple underwater air bubble manipulation system will open an easy and cheap protocol to address the inherent air bubble issue present in most of microfluidics applications or underwater surfaces (e.g. electrodes) without integrating any advanced tools or processes.

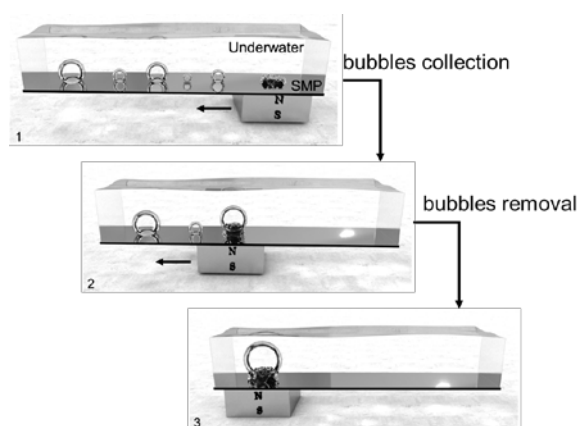


Figure 1. Schematic diagram of the magneto collection and removal of air bubbles in solid-water interface.

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Impact of the Ligand Shell on Structural Change and Decomposition of All-Inorganic Mixed-Halide Perovskite (CsPbX₃) Nanocrystals under X-Ray Illumination [1]

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The urge to find new materials that support the currently ongoing transformation process concerning energy consumption and production drives material science. Lead halide perovskites could play an important role in this. In solar cells lead halide perovskites show power conversion efficiencies up to 29 % [2]. Besides this application, perovskites also have the potential for the usage as scintillators, as they have already shown good performance in X-ray detection [4]. However, the instability of perovskite-based materials is a significant drawback for their application in optoelectronic and scintillating devices. Especially the often-reported process of photodegradation, exemplarily shown for the intensively studied methylammonium lead iodide (MAPbI₃) [3] and more recently also observed for mixed-halide cesium lead perovskites (CsPbX₃) [5], hinders the commercialization of perovskites. We will present our work on two model systems namely CsPbBrI₂ and CsPbBr₂Cl nanocrystals. We combined the results of two different methods that both utilize continuous X-ray irradiation. By exploiting wide-angle X-ray scattering (WAXS) experiments, we found a contraction of the atomic lattice during irradiation that can be correlated to a shift in core level electron binding energies observed in X-ray photoelectron spectroscopy (XPS) experiments. Our XPS studies reveal that the decomposition mechanisms under illumination strongly depend on the ligand shell of the perovskites. We will present the stabilizing effect of zinc-(5-monocarboxyphenyl-10,15,20-triphenylporphyrin) (mZnTPP) in comparison to the widely used oleic acid/oleylamine system.

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Synthesis, optical and structural properties of lead bromide perovskite nanocrystals for lighting emitters devices

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All-inorganic and organic-inorganic lead halide perovskite nanocrystals (NCs) based on bromide with the general formula of APbBr₃, in which A can be a metal cation such as cesium (Cs⁺), or an organic alkyl cation such as methylammonium (CH₃NH₃⁺; MA⁺) or formamidinium (CH(NH₂)₂⁺; FA⁺), are very promising high-color purity light emitters due to their pure green emission and excellent optical properties[1,2]. In this present work, Cesium, methylammonium, and formamidinium lead bromide (CsPbBr₃, CH₃NH₃PbBr₃, and CH(NH₂)₂PbBr₃) perovskite nanocrystals were synthesized by hot injection method according to M. Imran et al synthesis approach in which the benzoyl bromide was used as halides precursors [3]. The injection of the benzoyl bromide at the desired temperature, into a solution of metal cations with the proper ligands, triggers the nucleation and the growth of lead bromide perovskite NCs within a few seconds. By precisely tuning the relative amount of cation precursors (cesium carbonate and lead acetate for Cs-perovskite; formamidinium acetate and lead acetate for FA-perovskite; and methylamine and lead oxide for MA-perovskite), ligands (oleylamine and oleic acid), solvents (octadecene), benzoyl bromide, and the injection temperature (170°C Cs-perovskite, 75°C for FA-perovskite, 65 °C for MA-perovskite), we have been able to synthesize inorganic and organic-inorganic lead bromide perovskite APbBr₃ NCs with very monodisperse colloidal nanocubes with excellent control over the size distribution, very high phase purity, and excellent optical properties such as a high green photoluminescence emission with narrow full width at half-maximum, with PLQY as high. The resultant APbBr₃ lead bromide (NC) perovskite nanocrystals exhibit important structural and optical properties, which are among the best characteristics for a device emitting pure green light.

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Expansion of the InGaAs spectral response with HgTe nanocrystals

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In the short-wave infrared (SWIR), The InGaAs technology is the leading one, combining high carrier mobility, high homogeneity and complete control over *n-to-p* doping. Though highly performing, they also face limitations such as limited spectral tunability, prohibitive cost and complex coupling to the read-out circuit. Over recent years, significant progresses have been made in the development of nanocrystal-based detectors for infrared sensing. They offer several advantages such as their cost-effective and easy fabrication, their size-tunability over a wide infrared spectral range and their direct coating on electronics. Here, rather than pitting these two materials against each other, we design a heterostructure where HgTe nanocrystals are used to spectrally broaden the InGaAs photoresponse (up to 2 μm) while lifting the lattice matching constraints. The synergistic duo is built in a diode geometry in which *p*-type HgTe NCs are coupled to *n*-type InGaAs wires that are used as high mobility ($\mu > 1000 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$) minority carrier extractors. This paper establishes that efficient optoelectronic coupling can be made between colloidal and epitaxially grown materials.

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Ultrafast Transient Pump-Pump-Probe Spectroscopic Investigations on Seeded Nanorods

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Colloidal nanomaterials have been at the core of intensive research due to their interestingly tunable properties. These materials are full of potential, as their band-gaps can be varied; these materials offer their use in optoelectronic devices such as FET, solar cells, LED.² Another potential application of these nanomaterials is light-driven photocatalytic reactions such as clean H₂ production or CO₂ reduction.³ As a result of intense research efforts of the past decade, we can now reasonably control the morphologies of the nanomaterials and are now able to add reproducibly different components together to form so-called heterostructures. These heterostructures are of great interest as their band-gap positioning allows to spatially separate electrons and holes which enables us to extract them before recombining.

Metal-tipped CdSe seeded CdS nanorods have been widely explored nanoheterostructure for H₂ generation. Since photo redox reactions require multiple electrons to complete the reaction, understanding multiple electron dynamics in these systems is crucial to understanding the system thoroughly and derive structure-dynamics-function relationships. Ultrafast dynamics in CdSe@CdS dot-in-rod (DIR) nanoheterostructures can be tracked using transient absorption and time-resolved photoluminescence spectroscopy. Herein we introduced pump-pump-probe spectroscopy as a tool to gain insight into multiple exciton dynamics in heteronanostructures. The tunable color of repump allows us to selectively excite different moieties of the nanoheterostructure with a desired delay time. This technique enables us to observe the generation of multiple excitons in nanoheterostructures by consecutive absorption of photons and follow their dynamics. First proof of principle studies performed on CdSe@CdS DIR will be presented in this contribution.

Analysis of the conduction mechanism of the new nanomaterial Cu_2SnS_3 compound synthesized by hydrothermal route.

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The ternary compound semiconductors Cu_2SnS_3 , $\text{Cu}_2\text{ZnSnS}_4$ and similar chalcogenide materials can be used in solar cells owing to their high absorption coefficient [1]. Recently, the group of these kesterite has attracted much attention because of their important potential applications in photovoltaic cells. Among these ternary sulfides, Cu_2SnS_3 and Cu_3SnS_4 are the most promising compounds, and these can be used in sustainable solar cells due to their optimal direct band gap for solar energy conversion. The band gap of the Cu_2SnS_3 has been reported to be between 0.93 and 1.35 eV, which lies in an optimal region for photovoltaic application [2-4]. The study of the temperature and frequency dependence on AC conductivity, electric property and relaxation mode of this semiconducting materials have been extensively used to understand transport mechanism of charge carriers, which occurs through hopping between localized states. Electrical impedance spectroscopy (EIS) is considered to be a powerful tool of analyzing the electrical properties of polycrystalline materials [5]. Regarding the scientific innovation, the CTS nanoparticles were prepared using the hydrothermal synthesis. The present work reports some physical properties of Cu_2SnS_3 compound. The frequency and temperature dependencies of the AC conductivity and the electrical behavior have been investigated. By using the impedance spectroscopy this properties are studied in the high temperature range from 300°C to 440°C. Single contribution to total electrical conduction through the material is considered. Relaxation time was found to decrease with increasing temperature which follows the Arrhenius relationship.

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Time- and frequency-domain opto-electrical measurements on graphene at THz frequencies

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Graphene is still a promising candidate for future ultrafast, low-power-consumption information and communication technologies. Therefore, we investigate the optical-to-electrical conversion in graphene via time- and frequency-domain THz spectroscopy [1]. To this end, a Goubau-line circuit and a coplanar metal stripline in combination with an on-chip pump/probe scheme are used. The striplines act as highly sensitive near-field antennae with a bandwidth of up to 1 THz [2,3]. Our experiments clarify the optoelectronic mechanisms contributing to the photocurrent generation in graphene and at graphene-metal interfaces. [4].

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Cation Exchange on Single Semiconductor Nanowires

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The composition of nanostructures is of major importance for their properties. Changing the elemental composition while preserving the geometry of the nanostructure can be achieved by performing a cation exchange.

In my work, the exchange is investigated by converting single cadmium-sulfide nanowires to silver-sulfide nanowires. The cation exchange is studied by non-invasive optical and electrical methods. For the optical investigation, photoluminescence (PL) spectroscopy is conducted. The PL spectroscopy shows that the emission at 500 nm decreases with progressing cation exchange. Furthermore, it is expected that an emission peak around 1200-1300 nm is formed during the exchange originating from silver sulfide (bandgap: ~ 1.1 eV).

To investigate the electrical properties of the nanowires, nanowire-based field-effect transistors are fabricated *via* optical lithography. Charge-transport and transconductance measurements are carried out with these transistors. The charge-transport measurements show that the conductivity is increased on fully exchanged nanowires. Therefore, the cation exchange can be monitored and investigated with a minimum of interference in the reaction. Nanowires with carefully adjusted elemental composition, and thus adjusted electrical properties, could possibly find a way into electrical devices such as transistors or batteries.

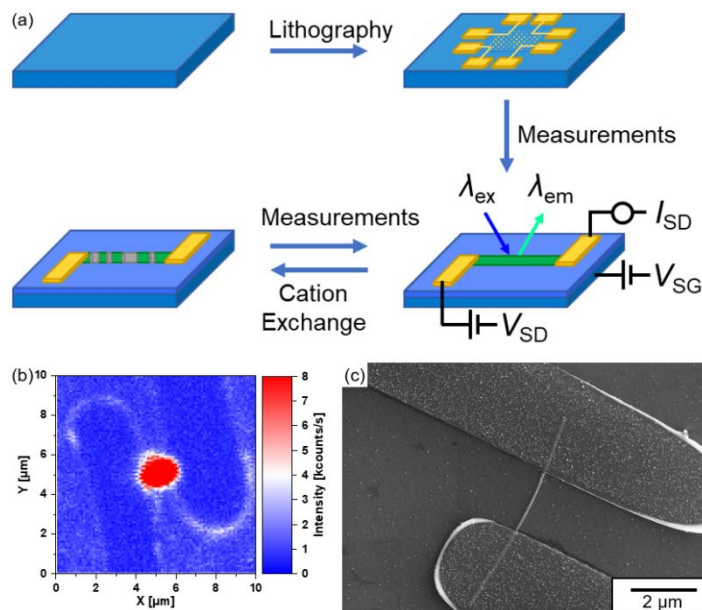


Figure 1: (a) Schematic overview of the work steps for the investigation of single nanowires, (b) PL-Scan and (c) SEM-Image of a contacted CdS nanowire.

Strongly anisotropic strain-tunability of excitons and Raman shift in exfoliated ZrSe₃ and ReS₂

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Applying mechanical deformations has become a powerful approach to modify the vibrational, optical, and electronic properties of two-dimensional (2D) materials.^[1] Different from 2D isotropic material, the effect of uniaxial strain along different crystal orientations is expected to modify the properties of these anisotropic 2Ds differently. Despite the recent interest on these families of anisotropic 2D materials, the number of reported research works focused on studying the effect of strain along different crystal directions is still very scarce, which activated our research interest on these 2D anisotropic materials.^[2-4]

Here we study the effect of uniaxial strain on the band structure of ZrSe₃, a semiconducting material with a marked in-plane structural anisotropy. By using a modified 3-point bending test apparatus, thin ZrSe₃ flakes were subjected to uniaxial strain along different crystalline orientations monitoring the effect of strain on their optical properties through micro-reflectance spectroscopy. The obtained spectra showed excitonic features that blueshift upon uniaxial tension, which is strongly dependent on the direction along which the strain is being applied, which shows a maximum when the flakes are strained along the b-axis. Ab initio calculations were conducted to verify this strain-tunable anisotropy on the excitons.

Apart from this, we also studied the strain-tunable vibrational property of ReS₂, it could be observed that a redshift with a maximum and a minimum gauge factor could be obtained when the strain is applied parallel and perpendicular to the crystalline orientation correspond to different Raman modes, respectively.

These works provide a better understanding of the role of strain on the properties of two-dimensional materials with a strong in-plane anisotropy and open an avenue for utilizing this strain-tunability on optical and electrical fields potentially.

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How does surface chemistry control the shape of semiconductor nanoplatelets?

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II-VI semiconductor nanoplatelets (NPLs) can crystallize in the cubic zinc blende crystal structure. Both, the orientation of these NPLs and their surface defined at the atomic scale induce the self-assembly of organic ligands over thousands of nm² on the top and bottom basal planes of these anisotropic nanoparticles [1]. NPLs curl into helices under the influence of the surface stress induced by these ligands. We can control the radii of NPLs helices through the ligands described as an anchoring group and an aliphatic chain of a given length. A mechanical model accounting for the misfit strain between the inorganic core and the surface ligands predicts the helices radii. It can be shown that the chirality of the helices can be tuned by the ligands anchoring group and inverted from one population to another [2].

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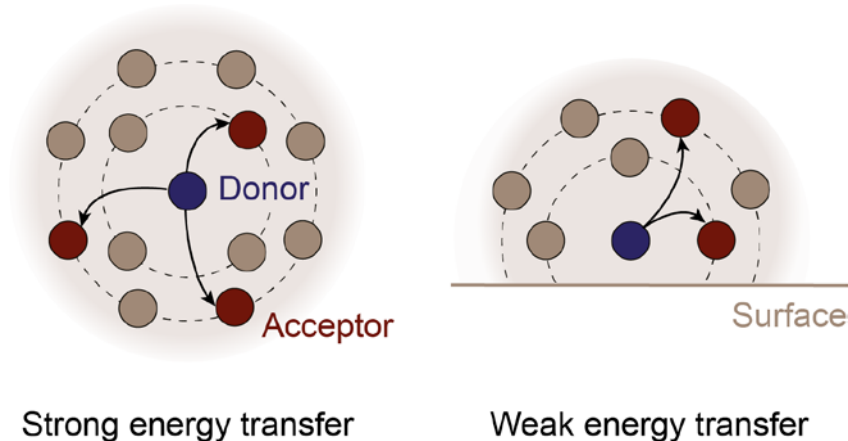
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Finite-size effects on energy transfer between dopants in nanocrystals

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Nanophosphors often rely on energy transfer between optically active dopant ions, so that one species absorbs light of one color and another species emits light of the desired color. As the relevant optical transitions are localized at individual atoms, it is generally assumed that the intrinsic properties of nanophosphors are independent of the size or shape of the host crystal—much unlike the case of semiconductor nanocrystals. Here, however, we show that finite-size effects do occur as the length scale of energy transfer is much larger than the atomic scale of the optical transitions.



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Nanowire based photovoltaic devices

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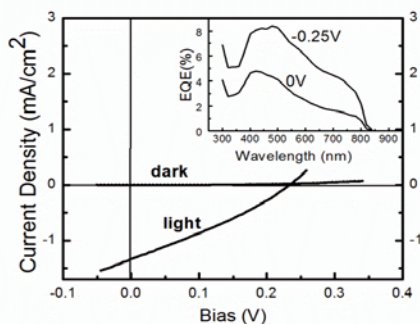
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With advanced state-of-the-art technologies, nanostructured materials are envisioned to offer promising potential for developing future photovoltaic devices with enhanced energy conversion efficiency. With the advantage over the thickness limitation in the traditional thin film configuration, we design core-shell structured photovoltaics based on quasi-1D nanowires, in which light absorption and charge collection are in orthogonal directions.

A simple approach is to do stepwise deposition into such template to make high-quality radial junctions at the core-shell interface. So far we have first studied core-shell nanostructured photovoltaics based on various nano templates, such as anodized TiO₂ nanotube arrays (ATO), anodized aluminum oxide (AAO) nano porous membranes and Si nanorod templates.

By electrodepositing CdTe into ATO template, core-shell CdTe/TiO₂ nanostructures with 1:1 stoichiometry as well as several prototype of solar cells have been successfully fabricated. Under AM 1.5G illumination, this solid-state solar cell yields an open circuit voltage of 0.23 V, a short circuit current density of 1.23 mA/cm² and a fill factor of 30%. Compared to the external quantum efficiency (EQE) measured at 0 V, the EQE under negative bias shows significantly higher values (as shown in the figure below), suggesting that even a higher photocurrent can be achieved by improving the carrier collection process.

Figure



I-V characteristic under AM 1.5 illumination of a CdTe/TiO₂ solar cell prototype. The inset shows the External Quantum Efficiency of the corresponding prototype at a bias of 0 V (a) and -0.25 V (b).

2D/1D MoS₂/TiO₂ Heterostructure with Wavelength-Dependent Charge Transfer Pathway for Selective Photocatalytic CO₂ Reduction

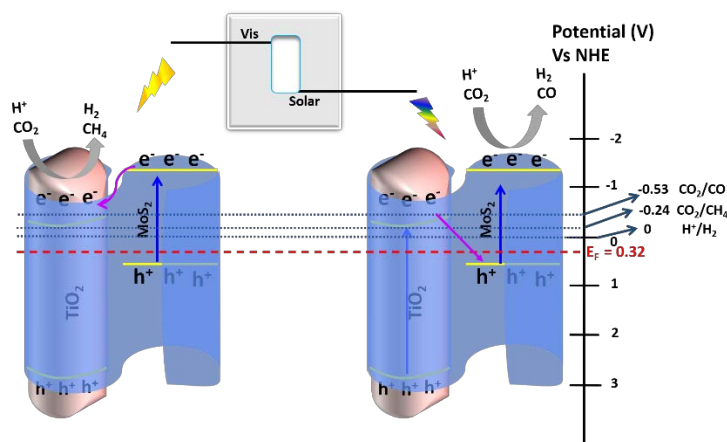
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Abstract

Regulating the transfer pathway of charge carriers in heterostructure photocatalysts is great of importance for selective CO₂ photoreduction. Herein, we succeed to regulate the charge transfer pathway and in turn the redox potential in a MoS₂/TiO₂ heterostructure by varying the light wavelength range. Several *in situ* measurements and experiments confirm that charge transfer follows either a Z-scheme mechanism under simulated solar irradiation or a heterojunction approach under visible light illumination, elucidating the switchable property of the MoS₂/TiO₂ heterostructure. Replacing the simulated sunlight irradiation with the visible light illumination switched the photocatalytic CO₂ reduction product from CO to CH₄. ¹³CO₂ isotope labelling confirmed that CO₂ is the source of carbon for CH₄ and CO products. This study opens a new window to develop photocatalysts with wavelength-dependent charge transfer pathway and redox potential for selective artificial photosynthesis.



Ultrafast Interactions in Dual-Plasmonic Core-Shell Au@CuS Nanoparticles

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Heterostructured Au-CuS nanoparticles (NPs) show two distinct localized surface plasmon resonances (LSPRs) in the visible and the near-infrared (NIR) range. These LSPRs are based on electrons in gold and holes in copper sulfide and do not appear to interact with each other at steady state. It is therefore both surprising and exciting that we have observed interactions using ultrafast transient absorption spectroscopy (TA). We measure a response of both regimes regardless which LSPR was excited by the laser pulse. A comparison with a mixture of Au-NPs and CuS-NPs shows, that this interaction only occurs in heterostructured Au-CuS NPs and doesn't extend over longer distances. Using a time-dependent fitting procedure, we reconstruct the spectral position, broadening, and amplitude of the LSPRs and can calculate the charge carrier densities of the electrons and holes in the respective regimes. We have found that both resonant and non-resonant excitation induce charge carrier densities after 800 fs in each regime, and decay via two first-order processes in either case. The rapid decay of $\tau = 1$ ps of the charge carrier densities after excitation is indicative for charge-phonon scattering. It is followed by a slower process of 30 ps to 40 ps which is typical for phonon-phonon scattering. Our findings deepen the understanding of multiplasmonic interactions in heterostructured nanoparticles and will propel applications where such interactions are essential, such as catalysis.

The effect of water intercalation into tungsten trioxide structure on photocatalytic properties: connectin between crystallographic structure and electronic properties.

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Tungsten trioxide continue to attract a lot of attention for its promising optoelectronic properties in photocatalysis[1], photo electrochemistry[2] and photochromism[3]. A particular interest was devoted to tuning its electronic structure and optical gap in order to enhance the photocatalytic performance in hydrogen production as well as in advanced oxidation process. One of the alternatives is the introduction of water molecule into tungsten oxide structure by intercalation reaction. In this communication, three varieties of tungsten trioxide: Tungsten oxide (WO_3), tungstite ($\text{WO}_3 \cdot \text{H}_2\text{O}$) and hydrotungstite ($\text{WO}_3 \cdot 2\text{H}_2\text{O}$) were prepared and characterized by PXRD, FTIR spectroscopy and reflectance spectroscopy. The structures of intercalated materials were refined using Rietveld method and the electronic proprieties such as gap energy, conduction band and valence band energies were estimated form UV-visible spectroscopy. The obtained results show that the introduction of water molecules into tungsten oxide structure reduces the gap energy from 3 eV to 2.46 eV for tungstite and 2.62 eV for hydrotungstite. These results were explained using crystallographic data that are suggesting the distances between two adjacent layers of WO_6 in tungstite and hydrotungstite are larger than in WO_3 which will lead to negative shift of the conduction band. Furthermore, the average W-O-W tilt angle in WO_3 is less important in comparison with $\text{WO}_3 \cdot 2\text{H}_2\text{O}$ and $\text{WO}_3 \cdot \text{H}_2\text{O}$. This result could be evidence that shed the light on new alternative of band-gap engineering through intercalation.

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Computational study of chalcopyrite-type nanomaterials for solar cell applications

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Study of transition-metals doped chalcopyrite-type nanomaterials has been attracting a lot of attention in recent years due to its numerous applications especially in solar cells, LEDs, photocatalysis and medical imaging. In this report, we have studied the structure and optoelectronic properties of CuTiY_2 ($Y = \text{S}, \text{Se}, \text{Te}$) by using Density Functional Theory. Our computed HOMO-LUMO gap is in the range of 1.993 eV to 2.620 eV. The result transpires a decrease of HOMO-LUMO gap with substitution of Ga by Ti in CuGaS_2 . It specifies that CuTiY_2 nanomaterials can be suitable candidate with enhanced electronic and optical properties for intermediate band gap material. The optical properties viz., refractive index, electronic polarizability, dielectric constant and optical electronegativity of these compounds are investigated. The result exhibits that compound with the maximum energy gap displays the least value of refractive index, electronic polarizability and dielectric constant, and vice-versa. Refractive index, electronic polarizability and dielectric constant of these compounds increase from S to Se to Te, whereas energy gap and optical electronegativity follow the reverse trend. The computed data are in well agreement with the experimental results.

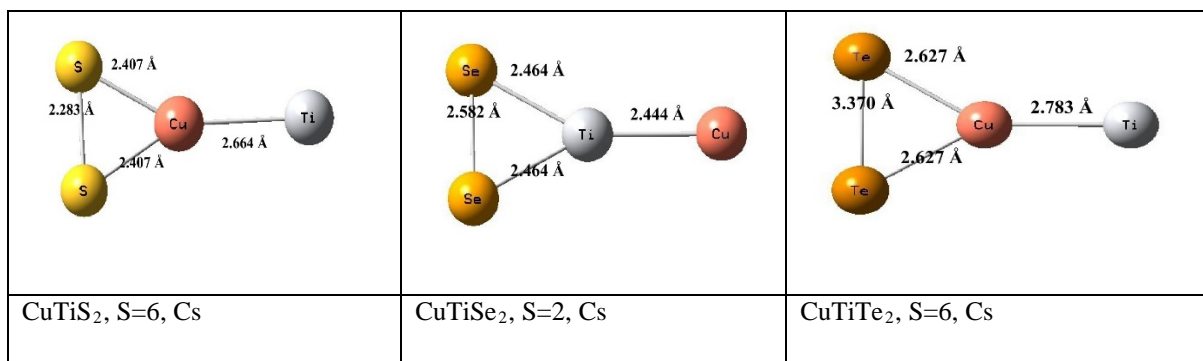


Figure 1: Ground state configuration of CuTiY_2

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Alkali metal modified fluorapatite as promising catalysts for biodiesel production

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Biodiesel, or fatty acid methyl ester (FAME), has emerged as an alternative fuel source since it exhibits similar physicochemical properties to conventional petroleum-based diesel. Unfortunately, the homogeneous catalytic process suffers from several drawbacks such as soap formation, tedious purification processes, corrosion of the reactors, production of large amounts of wastewater and difficulty to remove the catalyst after the reaction. However, the use of heterogeneous catalysts was used as an alternative to the several problems related to the homogeneous process. Many solid catalysts have been developed as potential catalysts for biodiesel production from vegetable, waste cooking oils and from fatty acids by transesterification and esterification reactions. Recently, many researchers have focused on the use of catalysts-based phosphates [1,2]. In this work we will present results about the use of fluorapatite modified alkali metals for biodiesel production. The obtained results showed that interesting yields of 1st and 2nd biodiesel generations could be obtained.

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Indium Tin Oxide (ITO) Nanocrystals Photo-doping: exploiting multiple-charge processes

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Within the new generation technology for energy progress, transparent conductive oxides are promising materials, with attractive high performances at low cost. This is especially true with the use of nanoparticles allowing the exploitation of solution processes. One of the best-known examples in optoelectronics are the Indium Tin Oxide (ITO) nanocrystals (NCs) [1]. Their properties, including light absorption in the ultraviolet range, the optical transparency in the visible and the infrared Plasmon resonance (LSPR), together with the nanofabrication turn these materials multifaceted and quite versatile. Concerning the energetic aspects the LSPR is crucial, being responsible for the conductive character thanks to the aliovalent doping [2]. Yet more recently, a further increase in charge density through a zero environmental impact treatment renewed the scientific interest for these materials. Many metal oxides nanocrystals demonstrated an exponential increase in charges through photodoping induced by multiple events of light absorption [3]. This phenomenon encourages even more the use of these inorganic semiconductors in a wide variety of energy-related fields such as photovoltaics, but also photo-electrochemistry and photo-catalysis. In each of these applications, one of the leading research lines concerns the analysis of the multiple charges accumulated through this light-driven method and the possibility of accessing processes involving multiple charge transfers. The consequences would be beneficial in particular in terms of efficiency. In this work [4], we report a first evidence, in the case of photo-doped ITO NCs, of the multiple-charge transfer process, counting in more than one electron, by means of a gradual oxidative treatment using an electron-acceptor molecule, the F4TCNQ. The spectroscopic analysis of the titration allows shedding light on the reactivity of the nanocrystals triggered upon illumination and on the potential transfer of multiple charges.

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Transient Absorption Spectroscopy of Colloidal 2D Transition Metal Dichalcogenides (TMDCs) at Cryogenic TemperaturesF.

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Ultrathin 2D transition metal dichalcogenides (TMDCs) exhibit interesting optoelectronic properties, high exciton binding energies and rich exciton physics [1]. Only recently, photoluminescent 2D TMDCs have been synthetically accessible by colloidal chemistry methods and open up new routes to e.g. heterostructures [2]. In order to understand ultrafast processes in colloidal TMDCs like the formation and recombination of excitons, we employ transient absorption spectroscopy (TAS). TAS is a pump-probe spectroscopy method where short (~100 fs) amplified optical laser pulses (pump) are used to photoexcite the sample. A time-delayed broadband “white light” continuum (probe) is used to study the nature, fate, and recombination of charge carriers at different times after the photoexcitation (500 fs up to 8 ns). Here, we describe our advanced experimental TAS set-up, which allows us to cryogenically characterize at liquid nitrogen or helium temperatures and discuss first results on the charge carrier dynamics of colloidal 2D MoS₂ layers.

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Photoluminescence polarization of an ensemble of arbitrarily oriented colloidal nanoplatelets

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Colloidal nanocrystals are promising nanoscale objects for applications in optoelectronics, biology, and medicine because they exhibit strong quantum size effects, demonstrate photostability, can be easily incorporated into other materials, and are inexpensive to synthesize [1]. Their long spin lifetimes open up the possibility of their employment in spintronics. Colloidal nanoplatelets, quasi-two-dimensional nanocrystals, in addition, possess atomically controlled thickness across the ensemble, regulated by synthesis conditions [2]. However, they exhibit lateral-size dispersion and possible in-plane anisotropy. This anisotropy leads to the splitting of the lower optically active exciton states into linearly polarized dipoles and affects the photoluminescent response to the linearly or circularly polarized excitation - effects of optical alignment and optical orientation.

An important feature of the ensemble of colloidal nanocrystals is their arbitrary orientation in the solution or on the substrate. Theoretically, we consider an ensemble of drop casted nanoplatelets with low enough concentration that each of them appears lying flat on the substrate, and arbitrary is its orientation in the plane.

When such an ensemble is illuminated with light of a certain linear polarization, each individual nanoplatelet can be regarded as a black box. The radiation coming out of this box in the magnetic field in Faraday geometry will to some extent preserve this linear polarization, rotate it, and convert to circular polarization. Averaging over the angle between one of the own nanoplatelet's dipoles and excitation polarization results in the absence of conversion of linear polarization into circular and vice versa in the experiment. The analysis of magnetic field polarization dependences allows us to estimate exciton spin lifetimes and energy structure parameters. Polarization conversion can be observed experimentally in an oriented ensemble or single nanoplatelet.

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Exploring the limits of neat MoS₂ photodetectors

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Using 2D-Materials like transition metal dichalcogenides (TMDCs) is the next step in order to produce fast and low switching energy photodetectors. For high frequency applications, tuning of the rise time is important since it determines the bandwidth of the whole device. Many approaches try to enhance the rise time of TMDC devices by creating heterojunctions with other TMDCs or 2D-materials like graphene. Within this work, only neat/pure MoS₂ is used and its response time optimized. To this end, one-dimensional 'edge on' contacts are fabricated to lower the contact resistance at the electrode/material interface as well as the characteristic transfer length. Additionally, the channel lengths as well as the active area over which the carriers are generated are reduced with electron beam lithography. Furthermore, the electrode geometry is changed to a bowtie structure to provide not only a small active area and short distances but also a plasmonic resonance. Due to this tuneable plasmonic behaviour, the electric field gets enhanced by orders of magnitude within the bowtie gap. All these lithographic steps lead to an acceleration of the rise time and, thus, a faster response of neat MoS₂ photodetectors. The concepts used can be transferred onto other materials as well and are not exclusively valid for TMDCs.

Insights into colloidal 2D MoS₂ nanosheet formation

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Two-dimensional (2D) transition metal dichalcogenides (TMDCs) exhibit highly interesting optoelectronic properties including strong spin-orbit coupling^[1], successive opening of the indirect band-gap with decreasing layer thickness down to the monolayer with a direct band-gap^[2], and a near-unity photoluminescence quantum yield^[3]. Ultrathin molybdenum disulfide (MoS₂) represents a promising candidate for investigation due to the potential fields of application ranging from sensors, nanoelectronics, superconductors and energy harvesting to catalysis. MoS₂ nano sheets are particularly interesting as the system has been studied thoroughly and its optoelectronic properties are well understood already. In literature the main synthetic routes for TMDC nanosheets are exfoliation and chemical vapor deposition methods^[4].

Here, using a colloidal synthesis pathway, we present a versatile alternative synthesis route for ultrathin TMDC nanosheets with tunable morphology, lateral size and ligand chemistry, as well as the characterization of the nanosheets with respect to their size and crystal phase. The characterization of the samples is carried out by applying scattering-corrected absorption spectroscopy, XRD, TEM and XPS.

Our results demonstrate how to control the formation of a specific MoS₂ nanosheet phase (semiconducting or metallic), by applying kinetic or thermodynamic reaction parameters, as well as the nanosheet size.^[5, 6]

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Enormous Artifacts in Luminescence Nanothermometry

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Knowledge of temperature on the smallest scale is becoming increasingly important since industry is pushing product dimensions to the nanoscale. Ratiometric nanothermometry can probe the temperature on these small dimensions using two emission lines of luminescent nanoparticles. For application of such nanoparticles as thermometers, the temperature is often assumed to be the only external parameter affecting the emission lines. In this work we observe enormous errors in temperature measurements using lanthanide-doped nanoparticles due to the photonic nano-environment. We systematically place these nanoparticles near a metallic reflector, varying the separation between 0 and 600 nm. We find errors of $\Delta T = \pm 50$ K for using the emission lines at 520 nm and 540 nm from thermally coupled states in Er³⁺-doped NaYF₄ nanocrystals. Thermometry with Ho³⁺-doped NaYF₄ nanocrystals, which emission lines at 545 nm and 650 nm, result in errors up to $\Delta T = \pm 200$ K. Both errors can be reproduced with a simple self-interference model. Such large temperature errors due to the photonic nano-environment can be detrimental for reliable thermometry in real-life applications and may be minimized by choosing a thermometer with emission lines with minimal relative frequency difference $\Delta\omega/\bar{\omega}$.

Kelvin probe force microscopy of nanostructures

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Kelvin probe force microscopy (KPFM) is a method of measuring the surface potential of a sample. Because it is based on atomic force microscopy (AFM), KPFM enables the investigation of nanostructures with a lateral resolution down to 25 nm and a potential resolution of 5 meV. Such nanostructures can be semiconductor nanowires, nanosheets or nanorods. These materials can be optically excited, showing charge separation or photoluminescence (PL). This project aims to combine optical, electrical and surface potential measurements in one setup in order to investigate the charge separation in these materials and bring insight into the band bending at semiconductor-metal interfaces.

KPFM is employed by applying an AC voltage to the cantilever of an AFM. The cantilever vibrates with the same frequency. A potential is applied to the cantilever which nullifies this vibration. The applied potential is equal to the contact potential difference, or the difference in work function between the tip and the sample. Nanostructures can be electrically contacted from both sides, and excited through transparent substrates. A confocal lens system allows for PL and exciton lifetime measurements. The transparent samples are made of ITO on which an insulating layer of silicon dioxide is sputtered. Additional gold contact patches can be applied using lithography. Nanostructures can be contacted by different metals, using electron beam lithography.

A CdS nanowire was contacted with gold and indium and a potential of 2 volts was applied to each side. It was shown that the potential drops differently along the wire depending on the direction of the bias. A reason could be that if the potential is applied to the indium electrode, the schottky contact of the gold contact is biased in reverse. If the potential is applied to the gold electrode, the schottky contact forward biased. It was shown, that KPFM is also capable of the investigation of CdS and CuS nanosheets, without excitation. On reduced graphene oxide it was shown, that the adsorption of isopropanol affects KPFM measurements.