# Uniting Today's Nanotechnology for Advancing Tomorrow's Semiconductor Physics

821. WE-Heraeus-Seminar

13 Nov - 15 Nov 2024 at the Physikzentrum Bad Honnef/Germany

The WE-Heraeus Foundation supports research and education in science, especially in physics. The Foundation is Germany's most important private institution funding physics.



#### 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 821. WE-Heraeus-Seminar:

This seminar discusses advances in the fabrication and optoelectronic properties of quantum-confined solid-state materials from the two viewpoints of bottom-up (e.g. wet-chemistry or molecular beam epitaxy) vs. top-down methods. The overarching hypothesis is that these communities, which currently act largely separately due to the different chemical approaches, face many identical physical challenges in the application of these nanomaterials for optoelectronics, such that an interdisciplinary exchange holds for a high degree of synergy.

With the advent of cryptocurrency mining, the wide-spread utilization of pretrained text generators and a superlinear growth in transmitted data volume, miniaturization of components for Information and Communication Technology (ICT) is a major challenge for semiconductor physics. It is anticipated that the world-wide electricity consumption due to ICT will exceed 10% in 2025, which requires major improvements in the energy efficiency of their key components to balance the growing demand for ICT applications with its energy consumption. Nanotechnology and the fabrication of device components with spatial confinement in one, two or even three dimensions has been at the forefront of providing solutions to this challenge. The seminar will focus on transport and optics in nanomaterials, detail characterization techniques and provide insights into a theoretical understanding and modelling of nanoscalic materials. While most materials of relevance in the context are semiconductors, the seminar will also include plasmonic nanomaterials, for instance to improve semiconducting applications by electromagnetic field enhancement. The overall goal of the seminar is to unite the top-down with the bottom-up nanofabrication community to jointly develop nanotechnological solutions for a faster and more energyefficient device physics of the future.

#### **Scientific Organizers:**

Prof. Dr. Christian Klinke	University of Rostock and Swansea University, UK E-mail: christian.klinke@uni-rostock.de
Prof. Dr. Marcus Scheele	Universität Tübingen, Germany E-mail: marcus.scheele@uni-tuebingen.de

# Introduction

## Administrative Organization:

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<u>Venue:</u>	Physikzentrum Hauptstrasse 5 53604 Bad Honnef, Germany Conference Phone +49 2224 9010-120 Phone +49 2224 9010-113 or -114 or -117 Fax +49 2224 9010-130 E-mail gomer@pbh.de Internetwww.pbh.de Taxi Phone +49 2224 2222
<u>Registration:</u>	Martina Albert (WE-Heraeus Foundation) at the Physikzentrum, reception office Tuesday (17:00 h – 21:00 h) and Wednesday (08:00 – 12:30 h)

## Tuesday, November 12, 2024

17:00 – 21:00 Registration

18:00 BUFFETT SUPPER / Informal get together

## Wednesday, November 13, 2024

07:45 – 08:45	BREAKFAST	
08:45 – 09:00	Scientific organizers	Opening and welcome
09:00 – 09:50	Keynote Iwan Moreels	Challenges and Opportunities for the Synthesis of Size-Controlled 2D Colloidal Nanoplatelets
09:50 – 10:10	Alireza Ghasemifard	Computational guide to optimize electric conductance in MoS <sub>2</sub> films
10:10 – 10:30	Dariia Matulka	Microscopic analysis of the energy density of quasi-2D crystals
10:30 – 10:45	COFFEE BREAK	
10:45 – 11:35	Keynote Klaus Ensslin	Quantum Devices in Graphene
11:35 – 11:55	Brindhu Malani Satya Seelan	Quasi-2D Ruddlesden-Popper nanoparticle-based photodetectors
11:55 – 12:15	James Caleb Peters	Fabrication of topological insulator Bi₂Se₃ Photodetectors for Photo Galvanic Applications
12:15 – 12:30	Conference photo	
12:30 – 14:00	LUNCH	

## Wednesday, November 13, 2024

14:00 – 14:50	Keynote Ivan Infante	Surface Reconstructions in Colloidal Quantum Dots
14:50 – 15:10	Rostyslav Lesyuk	Tuning of localized surface plasmons in natural hyperbolic copper chalcogenides CuX (X=S, Se)
15:10 – 15:30	K. David Wegner	Advanced nanomaterials for the short-wave infrared
15:30 – 16:00	COFFEE BREAK	
16:00 – 16:20	Zhouxiaosong Zeng	Ultrafast hot carrier cooling enabled van der Waals photodetectors at telecom wavelengths
16:20 – 17:05	Panel Discussion Panel Members : Klaus Ensslin Andreas Fery Iwan Moreels Christian Klinke Discussion leader: Marcus Scheele	The future of material development in (semiconductor) physics.
18:00 – 19:30	HERAEUS DINNER at the (cold and warm buffet, v	e Physikzentrum vith complimentary drinks)

19:30 POSTER SESSION I

# Thursday, November 14, 2024

08:00 - 09:00	BREAKFAST	
09:00 – 09:50	Keynote: Andreas Fery	Nanoparticle based materials: Opportunities and challenges
09:50 – 10:10	Florian Laible	Plasmonic nanostructures on flexible substrates
10:10 – 10:30	Lena Scholtz	Luminescent, Semiconductor Nanoparticle-Loaded Polymer Microbeads – Comparing Particle Architectures
10:30 – 10:45	COFFEE BREAK	
10:45 – 11:35	Keynote : Nahid Talebi	Phase-Locked Photon-Electron Interactions in Electron Microscopes
11:35 – 11:55	Daniel Lengle	Tracking Cation Exchange in Individual Nanowires via Transistor Characterization
11:55 – 12:15	Elshaimaa Darwish	Enhancing room temperature synthesis of lead halide perovskite and exploring its potential as a downshifting layer in solar cells
12:15 – 12:35	Christian Kuttner	Meet the Editor (of Nature Communications)
12:35 – 14:00	LUNCH	
14:00 – 14:50	Keynote : Caterina Cocchi	Discovery and characterization of complex materials using high- throughput ab initio methods
14:50 – 15:10	Zahra Shomali	Effect of non-local theory on precise investigation of heat transport in semiconductor nanostructures using non-Fourier macroscopic models

## Thursday, November 14, 2024

15:10 – 15:30	Kleopatra Papagrigoriou	Single Nanoparticle Charging Dynamics in the Gas Phase
15:30 – 15:50	COFFEE BREAK	
15:50 – 16:40	Keynote : Ute Kaiser	Findings from the happy marriage between low-voltage atomically- resolved TEM and low-dimensional materials
16:40 – 16:50	Two Flash Talks from Pos	ster Session I
16:50 – 17:30	Panel Discussion Panel Members : Ivan Infante Caterina Cocchi Ferry Prins Ute Kaiser Tobias Hertel Discussion leader : Christian Klinke	The future of material characterization and modelling in (semiconductor) physics
18:00 – 19:00	DINNER	

#### 19:00 POSTER SESSION II

# Friday, November 15, 2024

08:00 - 09:00	BREAKFAST	
09:00 – 09:50	Keynote : Monika Fleischer	Top-down fabricated optical antenna configurations
09:50 – 10:10	Yan Vogel	Solvation Shifts the Band-Edge Position of Colloidal Quantum Dots by nearly 1 eV
10:10 – 11:00	Keynote: Ferry Prins	Visualizing Energy Transport in Nanostructured Semiconductors
11:00 – 11:15	COFFEE BREAK	
11:15 – 12:05	Keynote : Tobias Hertel	Charge-Carrier Interactions and Defect States in Semiconducting Carbon Nanotubes: From Excitons to Trions and Beyond
12:05 – 12:15	Two Flash Talks from Pos	ster Session II
12:15 – 12:30	Scientific organizers	Poster Awards and Concluding Keynote
12:30	LUNCH	

End of seminar and departure

Posters

	Posters I
Enrique Arevalo Rodriguez	Using scattering microscopy to characterize semiconductor materials
Maximilian Black	Long-range self-hybridized exciton polaritons in two-dimensional Ruddlesden- Popper perovskites
Amalia Coro	Exploring Low Dimensionality in Perovskite Materials
Antonella Cutrupi	Visualizing the energy transport of Perovskite Quantum-Dot Networks
Upasana Das	Enhanced Wide-Field Transient Photoluminescence Microscopy Using Fast- Gated ICCD for Carrier Transport Studies
Riya Dutta	Enhancement of Photoresponsivity and Broadband Detection Enabled by Upconverted CdSe Quantum Dot-Decorated Nanoporous MoS <sub>2</sub> .
Katharina Gerber	Time-resolved photocurrent spectroscopy on gold nanorods
Maximilian Grimmer	Boosting the magnetic response of a composite nanostructure in the optical region with a Fano resonance
Yan Yan Grisan Qiu	Ligand-Induced Structural Modulation on Nickel Redox States in 2D Metal-Organic Frameworks
Olga Guselnikova	Wet synthesis of 3D confined materials for plasmonic sensing and catalysis
Fagui He	Template Mediated Formation of Colloidal 2D SnTe Nanosheets and the Role of the Ligands

	Posters I
Carlo Höhmann	Simulation of Charge-Carrier Transport in Cadmium Sulfide Nanowires
Girish Kakkepalya Hanumantharaju	Ligand-dependant charge carrier dynamics in perovskite nanocrystal LEDs with polar electron transport layer
Adnan Kareem	Fabrication and Characterization of Iron Titanate Thin Films as a Potential Tunnel Barrier for Magnetic Tunnel Junction (MTJ's)
Gyulnara Khachartryan	Tailoring Quantum States in Coupled Cylindrical Quantum Dots through STIRAP
Gor Kharatyan	Exciton binding energy and interband absorption in a cylindrical quantum dot GaN/InxGa1-xN

# Posters II

Nicolas Albenge	Plasmonically Enhanced Solar Water Splitting with TiO₂/Au/Pt Nanoparticles in PDMS Sponges
Ezat Kheradmand	Development and Optimization of RoHS- Compliant In(As,P) Colloidal Quantum Dots for Enhanced Optoelectronic Devices
David Kovács	Controlling the photofunctional properties of heterostructured Cu <sub>2</sub> O/Au nanoparticles by the arrangement of gold
Pannan Kyesmen	Tuning the surface properties of CuO films using the precursor aging approach for enhanced photoelectrocatalytic reactions
Sanaa Lahlali	A Comparative study of pressure effect on the structural, electronic and optical properties of LaXO <sub>3</sub> (X = Al, In, Ga) for Optoelectronic Applications
Lukas Lang	Surface Lattice Resonances in Plasmonic Gold Nanocone Arrays
Fedor Lipilin	An investigation into the potential of lanthanum oxide halides as gate dielectric materials in transistors
Mario Martin	Plasmonic nanoantennas for boosting TMDC based photodetection
Simone Mearini	Engineering the Electronic and Spin Configuration in 2D Metal-Organic Frameworks through Transition Metal Core Selection
Salma Naimi	Unveiling γ-Cul as a Promising Hole Transporting Material: A DFT Investigation for Enhanced Perovskite Solar Cells

	Posters II
Ronja Piehler	Space- and Time-Resolved Mapping of the Charge Carrier Diffusion in Nanostructured Organic-Inorganic Perovskites
Ifra Saeed	Electrodeposited Zirconium Titanate Thin Films: Structural, Magnetic, and Dielectric Properties for Spintronic Applications
Kalyan Jyoti Sarkar	Layered metal thio (seleno) phosphates for broad-band optoelectronics
Syed Abdul Basit Shah	Mn-Doped CsPbBr <sub>3</sub> perovskites for Luminescent Solar Concentrators and Photocatalysis
Melanie Sommer	Dielectric nanoantennas for optical studies on colloidal TMDC nanosheets
Lorenzo Tallarini	Exciton Dynamics in Perovskite Nanocrystal Superlattices with Different Interparticle Distance
Moritz Wehrmeister	Direct Observation of Hole Drift and Diffusion in Contacted Nanowires Under Local Illumination

# **Abstracts of Lectures**

(in alphabetical order)

# Discovery and characterization of complex materials using high-throughput *ab initio* methods

#### Caterina Cocchi

#### Institute of Physics, Carl von Ossietzky University Oldenburg

Ab initio methods have been gaining increasing importance in the characterization of existing materials and the prediction of new ones. The availability and success of these approaches has significantly boosted the development of complex semiconductors for applications in energy production, conversion, and storage. In this talk, I will illustrate how interfacing density functional theory with high-throughput screening routines can further enhance this potential, using as examples semiconducting materials currently used in particle accelerators [1,2], ternary oxides for lithium-ion batteries [3], and metal-organic frameworks [4,5]. Particularly, I will focus on the capability of high-throughput *ab initio* methods to assess the stability of particular configurations, to filter out unstable structures, and to accurately determine the electronic and spectroscopic properties of the selected ones.

#### References

[1] H.-D. Saßnick and C. Cocchi, J. Chem. Phys. 156, 104108 (2022).

[2] H.-D. Saßnick and C. Cocchi, npj Comput. Mater. 10, 28 (2024).

[3] T. Reents, E. Kataev, D. Duarte-Ruiz, R. Wilks, R. Garcia-Diez, M. Bär, and C. Cocchi, *submitted* (2024).

[4] H.-D. Saßnick, F. Machado Ferreira De Araujo, J. Edzards, and C. Cocchi, Inorg. Chem. **63**, 2098 (2024).

[5] J. Edzards, H.-D. Saßnick, J. Santana Andreo, and C. Cocchi, J. Chem. Phys. **160**, 184706 (2024).

# Enhancing room temperature synthesis of lead halide perovskite and exploring its potential as a downshifting layer in solar cells

#### Elshaimaa Darwish

University of Erlangen-Nuremberg (FAU), i-MEET institute WW6, Erlangen, Germany

Energy demands have kept increasing in recent years due to expanding human activity. Silicon solar cells offer an attractive renewable energy source while their external quantum efficiency (EQE) can still be enhanced; one way of doing this is by applying a photon energy downshifting layer. Herein, Cs4PbBr6 is applied as a downshifting layer; the Cs4PbBr6 is synthesized in the form of colloidal nanoparticles, and several modifications are introduced to the synthesis process, resulting in the enhancement of the photoluminescence quantum yield, improving the particle size distribution and reducing the CsBr impurities which appear as a side product during the synthesis of Cs4PbBr6. The application of the produced modified particles in the form of thin films on the top of Si solar cells shows an enhancement of the (EQE) of the solar cells when compared to the unmodified particles.

## **Quantum Devices in Graphene**

#### Klaus Ensslin

#### ETH Zurich, Physics Department, Switzerland

Graphene is a semimetal, but can become a semiconductor in case of bilayer graphene. The wide variety of physical phenomena of semiconductors, metals, and even superconductors can be implemented in various graphene structures. Highquality quantum dots can be prepared in gate-defined bilayer graphene. Spin, charge and valley states have been identified and lifetimes have been measured. When bilayer graphene is van der Waals bonded with a neighboring layer of TMD (transition metal dichalcogenide) effects of spin-orbit interactions can be observed when the wavefunction in the bilayer graphene is close to the TMD. For quantum point contacts we demonstrate situations where the spin-orbit splitting is comparable to the orbital level splitting and can be tuned by gate voltages. Also quantum dots can be realized in such gate-defined structures. Many of the techniques known for conventional quantum dots (Si, Ge, GaAs) can be applied to graphene quantum dots and give rise to unusual behavior of the level spectrum and its manipulation by gate electrodes.

We also discuss how superconducting structures based on magic-angle-twistedbilayer graphene can be used to build Josephson junctions, SQUIDs and to observe vortices entering and leaving the superconductor.

This work was done in collaboration with Jonas Gerber, Efe Ersoy, Christoph Adam, Artem Denisov, Wister Huang, Michele Masseroni, Max Ruckriegel, Hadrien Duprez, Lisa Gächter, Chuyao Tong, Rebekka Garreis, and Thomas Ihn.

## Nanoparticle based materials: Opportunities and challenges

#### Andreas Fery

Leibniz Institut für Polymerforschung Dresden e.V., Institute of Physical Chemistry of Polymers / Polymer Physics, Hohe Str. 6, 01067 Dresden

The assembly of nanoparticles is key for leveraging their unique properties for applications and even unlocking novel emergent properties via controlling local coupling processes, collective effects or metamaterial effects. I will discuss recent advances in the field with emphasis on the design of coreshell particles and emergent properties resulting from patterned particle assembly.

The ligand shell of particles plays a crucial role in the colloidal stability and assembly processes of particles. Polymeric ligands have shown advantages for particle assembly compared to low molecular ligands: A high concentration of ligands during the assembly process can be avoided as the adsorbed state is thermodynamically strongly favorable and inter-particle distances can be controlled via choosing appropriate molecular weight and polymer surface densities. However, their role can go beyond stabilization if electronically functional polymers are forming the nanoparticle shell and I will discuss examples of functional core-shell nanoparticles as well as developments in the coupling chemistry and its impact on optoelectronic properties.

Patterned assembly of nanoparticles adds a level of complexity but as well provides unique options for achieving emergent properties. There are many examples from the area of plasmonic nanoparticles such as surfaces featuring field enhancement effects for sensing or metamaterial effects such as giant circular dichroism metasurfaces. Patterned assembly of semiconducting nanoparticles has so far received less attention and I will discuss recent results on patterned assembly of quantum dots and perovskites giving rise to reduced lasing threshold and directional photoluminescence.

Finally, I will discuss options of particle based materials for circular economy approaches for electronic/optical devices.

## **Top-down fabricated optical antenna configurations**

### M. Fleischer<sup>1</sup>

<sup>1</sup>Institute for Applied Physics and Center LISA+, Eberhard Karls University Tübingen, Tübingen, Germany

While bottom-up nanofabrication techniques potentially allow for preparing large quantities of nanoparticles with ultra-high precision, top-down strategies enable the creation of nanostructures with a larger choice of pre-defined geometries at specific positions and in pre-designed configurations. Over the last few decades, a wealth of techniques and dedicated instrumentation for top-down nanofabrication has been developed. Most commonly, electron or focused ion beam lithography is employed in nano-optics research to prepare individual nano-antennas with tailor-made optical properties. An introduction to different top-down fabrication approaches will be given, and examples for the preparation of plasmonic nanostructures will be shown. Sample implementations of nano-antennas integrated with semiconducting nanomaterials and the resulting modified opto-electronic properties of such hybrid systems will be demonstrated. Specifically, the modified emission properties of semiconducting quantum dots coupled to nano-antennas and the strong light-matter-interaction of nano-antenna gratings within organic thin films will be highlighted.

Contributions by past and present group members are gratefully acknowledged.



Figure 1: (a) Sample SEM images of (mostly) top-down fabricated nano-antennas (see e.g. [1-6]); (b) schematic of a bright directional single-photon source [7]

- [1] W. Tao et al., Adv. Photonics Res. 4, 2300012 (2023)
- [2] S. Dickreuter et al., Nanophotonics 7(7), 1317 (2018)
- [3] F. Laible et al., Nanophotonics 9(6), 1391 (2020)
- [4] F. Laible et al. Nanoscale **10**, 14915 (2018)
- [5] A. Horrer et al., Anal. Bioanal. Chem. 407(27), 8225 (2015)
- [6] C. Dreser et al., Nanoscale 11, 5429 (2019)
- [7] H. Abudayyeh, ACS Nano **15**(11), 17384 (2021)

# Impact of edge termination and layer overlap on vertical and lateral electron transport in bilayer MoS<sub>2</sub>

Alireza Ghasemifard<sup>1</sup>, Agnieszka Kuc<sup>2,3</sup> and Thomas Heine<sup>1,2,3</sup>

<sup>1</sup>TU Dresden, Theoretical Chemistry, Bergstr. 66c, 01062 Dresden, Germany <sup>2</sup> Helmholtz-Zentrum Dresden-Rossendorf, HZDR, Bautzner Landstr. 400, 01328 Dresden, Germany

<sup>3</sup> Center for Advanced Systems Understanding, CASUS, Conrad-Schiedt-Straße 20, 02826 Görlitz, Germany

Molybdenum disulfide (MoS<sub>2</sub>) has a great potential in nanoelectronic applications, especially when thinned to a few layers. Liquid phase exfoliation enables large-scale fabrication of thin films comprising single- and bilayer flakes of MoS<sub>2</sub> and other transition-metal dichalcogenides (TMDCs), exhibiting variations in flake size, geometry, edge terminations, and overlapping areas. Electronic conductivity is thus determined by two contributions: the intraflake conductivity, reflecting the value of each single layer, and electron transport across these overlapping flakes. Employing first-principles simulations, we investigate the influence of overlap between flakes and various edge terminations on the electron transport between layers of MoS<sub>2</sub>. Our findings reveal the presence of electronic edge states, resembling donor and acceptor states in doped semiconductors, originating from the edge atoms and their chemical environment. We demonstrate that selective control over the dominant charge carrier type (n-type or p-type) can be achieved by tuning the gate bias. This bias modulates the occupation of edge states, leading to either electrons or holes as the majority carriers. Notably, pristine zigzag Mo-edge exhibits constructive interference and high conductance, whereas pristine zigzag S-edge displays destructive interference and low conductance. Mo-edge under the S-rich condition preserves the constructive interference pattern, albeit with a slight decrease in conductance. Increasing the overlap length between flakes from ~1 to ~23 enhances quantum conductance in the range of 20% to 44% across different edge configurations, indicating the degree of layer overlap as another important factor defining the efficiency of electron transport. These insights should be general for other TMDC semiconducting layers and are important for optimizing the design of TMDC-based nanodevices, offering pathways for developing efficient transistors.

## Charge-Carrier Interactions and Defect States in Semiconducting Carbon Nanotubes: From Excitons to Trions and Beyond

### Tobias Hertel

Institute of Physical and Theoretical Chemistry, JMU Würzburg, Germany

Semiconducting single-wall carbon nanotubes (s-SWNTs) exhibit a rich spectrum of optical phenomena, underpinned by strong Coulomb interactions and lowdimensional confinement effects. While excitons and trions are often at the forefront of discussions on the photophysics of s-SWNTs, recent work has shown that a diverse range of other optical excitations can arise due to localized defects, charge-carrier interactions, and electron-phonon coupling [1-4]. This presentation will provide insights into some of the intricate optical phenomena in pristine, doped, and chemically functionalized s-SWNTs, observed when using linear and nonlinear spectroscopies.

Among other findings, our recent studies have illuminated the role of charge carrier localization induced by Coulomb interactions with exohedral charges, leading to phenomena such as Fano-like resonances, exciton band shifts, and enhanced trion formation. At low doping levels, these effects manifest in non-radiative decay pathways dominated by exciton migration to localized defect states, while at higher concentrations, decreasing charge separations give rise to coupling between impurity states, as evidenced by electron paramagnetic resonance.

A comprehensive understanding of these effects is crucial not only from a fundamental perspective but also for advancing their application in next-generation optoelectronic devices in low-dimensional semiconductors. By combining spectroscopic results with microscopic modeling, we therefore have explored how the characteristics of Coulomb defects can be tuned by dielectric screening, effective band masses and nanotube chirality. Our findings provide new perspectives on how excitonic and trionic states may be modulated by covalent and non-covalent functionalization, potentially unlocking new functionalities for s-SWNT-based device architectures [5].

- 1. Sperlich et al., JCP 160, 234702 (2024)
- 2. Eckstein and Hertel, JPCC 127, 23760 (2023)
- 3. Eckstein et al., JPCC 127, 19659 (2023)
- 4. Eckstein et al., ACS Nano 11, 10401 (2017)
- 5. Khasminskaya et al., Nature Phot. 10, 727 (2016)

# Surface Reconstructions in Colloidal Quantum Dots

<sup>1</sup>BCMaterials, Leioa, BasqueCountry, Spain

Despite significant progress in recent years in understanding the chemical reactions occurring on the surfaces of II-VI, III-V, and lead halide perovskite quantum dots (QDs), there are still fundamental questions that remain unanswered regarding the nature of QD surfaces and the formation of trap states. Addressing these aspects is crucial for enhancing the optoelectronic efficiency of QDs. To tackle these challenges, an essential step is the utilization of first principle simulations to analyze QD surfaces. Traditional simulations have been limited by their restricted system size, typically confined to a few hundred atoms, and their focus on static properties without considering dynamic effects.

In this study, we use DFT calculations to study the electronic properties of QDs as a function of size, up to a diameter of ~4.5 nm. We show that increasing the size of QD models traditionally used in DFT studies leads to the collapse of the band gap and localization of the HOMO and LUMO levels on facet-specific regions of the QD surface. The introduction of surface vacancies with specific patterns leads to surface reconstructions that widen the band gap and delocalize both the HOMO and LUMO. These results show that the surface geometry of the facets plays a pivotal role in defining the electronic properties of the QD.

#### References

[1] J. Llusar, I. du Fosse, Z. Hens, A. Houtepen, I. Infante, ACS Nano, 18, 1563-1572 (2024)

## Findings from the happy marriage between low-voltage atomically-resolved TEM and low-dimensional materials

#### Ute Kaiser

Institute for Quantum Optics, Ulm, Germany

Graphene and other 2D matter, although being rather new materials, have already taken a firm place not only in research but also in application. That this development could proceed so fast is also the result of the practical realization of aberration correction so that low-voltage atomically-resolved TEM/STEM could become reality. Not only the structure but physical and chemical properties of these low-dimensional material can now be determined on the level of a single atom. We can summarize in one sentence: Low-dimensional materials and lower-voltage atomically-resolved TEM/STEM are just made for each other.

We begin our discussion by deriving fundamental understanding of the interaction of the lower energy electron beam with the 2D inorganic crystal from atomically resolved, voltage-dependent TEM images using the chromatically and spherically aberration-corrected low-voltage SALVE instrument. We discuss specifics of sample preparation of our 2D materials. We then utilize the electron beam for atomically-resolved structural imaging and modification of various 2D TMDs and TMPTs arranged in a Janus structure as well as in lateral and vertical heterostructures. We further demonstrate proof-of-principle experiments in which defect-characterized TMD flakes are transferred from a TEM grating to arbitrary substrates and relate the subsequently measured photoluminescence and transport signals to the defect structure.

Knowledge gained from the study of 2D inorganic materials is applied to the study of 2D polymers and 2D metal-organic frameworks (MOFs), however, atomicallyresolved imaging is hindered due to much lower resilience during electron irradiation. We present key strategies to achieve higher resolution in high-resolution TEM images of 2D polymer films. Finally, basics finding are presented such as the bonding nature between two atoms.

## Acknowledgement

We are grateful for the financial support of the German Research Foundation (DFG) and the Ministry of Research, Science, and Arts Baden-Württemberg (MWK) within the SALVE Project. The financial support of the German Research Foundation (DFG) within the DFG projects #456681676, #426572620, #464283495 is acknowledged. The financial support of the European Research Commission (ERC) within the Flagship "Graphene" (Core 2 and 3) is acknowledged.

## **Plasmonic nanostructures on flexible substrates**

#### <u>F. Laible<sup>1</sup>, W. Tao<sup>1\*</sup> and M. Fleischer<sup>1</sup></u>

<sup>1</sup>Institute for Applied Physics and Center LISA+, Tübingen, Germany \*now at: Dongguan University of Technology, Guangdong, China

Plasmonic nanoantennas are metal particles smaller than the wavelength of visible light. They can be excited optically or electronically. This results in both cases in a high near field and light emission at their resonance frequency. Two or more nanoparticles in proximity can couple to each other, leading to mode hybridization, which is highly sensitive to the interparticle distance.

The introduction of flexible support materials for the nanostructures enables more research areas like strain sensors, studying the coupling of individual nanoantennas, or testbenching optomechanical effects. The direct fabrication of plasmonic nanoantennas on flexible substrates is challenging. In most cases, a transfer process is used, where the nanostructures are prepared in a top-down process on a sacrificial layer. Afterward, the flexible substrate is placed on top, and the sacrificial layer is dissolved, thus transferring the nanostructures.

Variations of this process are used in the first two parts of this contribution. Firstly, rings fabricated on flexible Polydimethylsiloxane (PDMS) substrates will be shown. By stretching the substrate, a deformation of the rings is detected in their spectra and electron microscope imaging. The altering of the ring shapes that are introduced is dependent on ring thickness and overall structure size [1]. Secondly, bow tie nanostructures with small gaps are fabricated on PDMS substrates. The substrates are stretched unidirectionally. Depending on the orientation of the nanostructures to the strain direction, the bow tie gap increases or decreases significantly, changing the plasmonic coupling. A minimal gap size in the single-digit nanometer regime could be realized by improving the minimal gap size achievable with the electron beam lithography device resist combination [2].

In the third part of the presentation, a different kind of mechanically tunable system will be introduced. To reduce the gap in a bow tie nanostructure to the sub-1 nm regime, a nanoantenna is integrated into a break junction. As a flexible substrate, stainless steel sheets covered with Polyimide are used. The break junction is prepared by top-down e-beam and UV lithography. Optomechanical measurements with bow tie gaps well into the tunneling regime reveal an increase in tunneling current when the tunnel junction is illuminated by the laser of the confocal microscope [3].

- [1] W. Tao, Nano Convergence **10** (1), 15 (2023)
- [2] F. Laible, Nanoscale **10** (31), 14915 14922 (2018)
- [3] F. Laible, Nanophotonics 9 (6), 1391 1400 (2020)

## Tracking Cation Exchange in Individual Nanowires via Transistor Characterization

## Daniel Lengle<sup>1,2</sup>, M. Schwarz<sup>1</sup>, S. Patjens<sup>1,3</sup>, M. E. Stuckelberger<sup>3</sup>, C. Ruhmlieb<sup>1</sup>, A. Mews<sup>1,2</sup>, A. Dorn<sup>4</sup>

 <sup>1</sup>Institute of Physical Chemistry, University of Hamburg, 20146 Hamburg, Germany
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The properties of nanostructures are largely determined by their material composition and their geometry. Chemical cation exchange reactions allow a controlled change of the elemental composition within a nanostructure while preserving its geometry.

However, controlling the exchange at the single particle level is challenging. Here, we investigate the successive cation-exchange with silver on individual semiconducting nanowires. For this purpose, nanowire field-effect transistors are fabricated via optical lithography. These devices are characterized by atomic force microscopy to obtain key parameters such as nanowire diameter and channel length. Cation exchange is then performed by immersing the device in a silver nitrate solution. By precisely timing the duration in the solution, the reaction progress and thus the exchange degree can be controlled. Transport measurements reveal a change in conductivity, charge carrier concentration, and mobility.<sup>[1]</sup>

We prove that the cation exchange can be monitored and studied with a minimum of interference in the reaction. Nanowires with carefully adjusted elemental composition, and thus adjusted optoelectronic properties, may find their way into electrical devices such as sensors, transistors or batteries.

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## Tuning of localized surface plasmons in natural hyperbolic copper chalcogenides CuX (X=S, Se)

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Hyperbolic materials are known to have fascinating optical properties and can exhibit such effects as extreme light confinement, negative refraction, subdiffractional volume-confined polaritons, anomalous diffraction, photonic spin Hall effect etc. Among these materials, there is a family of so-called natural (homogeneous or single-phase) hyperbolic materials with strong intrinsic anisotropy and hyperbolic dispersion, i.e. the permittivity tensor has opposite sign along different axes. Graphite, tetradymites, ruthenates, hBN etc. belong to this class. Recently it was found that abundant and cost-effective copper sulfide (covellite) can demonstrate hyperbolic properties in the NIR region. This talk will focus on colloidal copper sulfide and selenide (klockmannite) nanocrystals both of which show hyperbolicity in the NIR region. Their optical properties are investigated in detail using both experimentally synthesized nanocrystals, and theoretical approaches including simple and complex-scaled DDA and DFT simulations.

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## Microscopic analysis of the energy density of quasi-2D crystals

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To create energy storage devices with a high energy capacity, materials with a high specific surface area for electrodes are required. Graphene and a number of quasitwo-dimensional crystals (q-2DCs), are characterized by such surfaces. Despite some differences between q-2DCs, all can be represented as packets of a set of monoatomic planes with covalent or ionic-covalent interatomic bonds, and interpacket bonds are realized by van der Waals (vdW) forces. The distance between adjacent packets or the vdW gap can be altered by various external factors. On the other hand, q-2DCs can be identified as porous materials. In such crystals, strictly spatially ordered vdW gaps of equal width play the role of pores. We propose a model that takes into account the defining characteristics of the q-2DCs. In it, the one-electron potential has the form  $V(\vec{r}) = V(x, y) + V(z)$ , where V(x, y) is the potential in the plane of the packets, and the potential V(z) along the normal to the packets has been chosen as the Kronig-Penney potential. In q-2DCs, the barriers describe packets and the wells describe vdW gaps. When the potential barrier is infinite, the dispersion law is a set of zones. The use of such a dispersion to calculate the energy density at different values of the parameters namely the applied voltage, the vdW gap at different values of the chemical potential.

Calculations of the energy density W based on the proposed microscopic theory show:

a) a significant relationship between the geometrical, spectral and statistical properties of the q-2DCs.

b) the presence of an experimentally established sharp maximum energy density at a small van der Waals gap;

c) indicates that there are more than two 'optimal' sizes of van der Waals gap. These are the sizes at which maximum energy density is achieved. The search for such maxima has been the subject of theoretical research by other authors, using a different set of assumptions.

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## Challenges and Opportunities for the Synthesis of Size-Controlled 2D Colloidal Nanoplatelets

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2D colloidal nanocrystals, also called nanoplatelets, offer great prospects to advance quantum dot-based applications such as light-emitting diodes or displays.[1] Compared to spherical 0D colloidal quantum dots, their uniform thickness, controlled on the monolayer level, yields narrower emission line widths, and their 2D shape allows for shorter emission lifetimes, as well as polarized emission in oriented films. In addition, 2D confinement of charge carriers strongly enhances the exciton binding energy,[2] which leads to stable excitons and even biexcitons at room-temperature. This expands the potential range of applications to for instance lasers or even quantum emitters.

However, advances in the synthesis of 2D nanocrystals with precise thickness and lateral dimensions have mostly focused on a model system consisting of 4.5 monolayer CdSe nanoplatelets. In this talk, I will discuss how to optimize the thickness, width and aspect ratio of various CdSe and CdTe nanoplatelets,[3-5] by controlling the size of the seeds during the nucleation via temperature and precursor reactivity, and the vertical and lateral growth kinetics via carboxylate or halide ligands. In addition, I will show how precisely controlled nanoplatelets are instrumental to improve our understanding of the fundamental properties of nanoplatelets, such as the exciton and biexciton binding energy, or can help to improve their optical characteristics, such as the fluorescence quantum quantum efficiency or optical gain coefficient.[6] Finally, I will give some examples of using the nanoplatelets in targeted photonic applications such as LEDs and scintillators.[7]

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## Single Nanoparticle Charging Dynamics in the Gas Phase

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Nanoparticles (NPs) exhibit unique size-dependent properties distinct from bulk matter due to shape, surface-to-volume ratio and quantum effects. These are already exploited in a multitude of applications involving heterogeneous catalysis, energy storage and optoelectronics. However, NP samples suffer from physical as well as chemical heterogeneity. This leads to a reduced performance in technological applications. Performance optimization requires obtaining insights into the intrinsic properties of individual NPs and how they contribute to the properties of the ensemble. Most single NP techniques, however, probe deposited particles, whose properties are perturbed, either by the support or neighboring particles. Probing truly inherent properties requires isolating a NP in the gas phase. Our approach to single NP characterization is based on guasi-continuous, non-destructive mass determination in a cryogenic split-ring electrode trap. Using this setup, we were able to demonstrate in situ fluorescence thermometry for semiconductor quantum dots as well as the feasibility of single NP action spectroscopy to measure UV/vis absorption spectra indirectly by monitoring adsorption/desorption of messenger molecules as a function of the irradiation wavelength.

For absolute mass determination and the quality of these long experiments (~ days), the ability to induce charge changes is crucial. To this end, we have characterized and achieved control over the charging and decharging (from 500 to 1200 charges) of single trapped, positively charged 100 nm diameter  $SiO_2$  and 50 nm diameter Au NPs. Electron attachment or charge transfer —mediated by different collision gases at different pressures— was induced by electrons emitted from a gauge filament. We examined the influence of the collision gas pressure, its ionization potential, and the initial charge state of the NP on the charging dynamics.

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## Fabrication of topological insulator Bi<sub>2</sub>Se<sub>3</sub> Photodetectors for Photo Galvanic Applications

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Topological insulators have attracted researchers' attention recently due to their unique surface states protected by time-reversal symmetry [1-3]. Since Bi<sub>2</sub>Se<sub>3</sub> has a low bandgap, it is expected to perform well in photodetection for visible and infrared optoelectronics [4,5]. Here, we present the preliminary results from our work on the growth, cleanroom fabrication, and characterization of Bi<sub>2</sub>Se<sub>3</sub> photodetectors. The Bi<sub>2</sub>Se<sub>3</sub> was grown on a sapphire substrate by Molecular beam epitaxy (MBE). The Raman modes at 72 cm<sup>-1</sup>, 132 cm<sup>-1</sup>, and 175 cm<sup>-1</sup> correspond to the A<sup>1</sup><sub>1g</sub>, E<sup>2</sup><sub>g</sub>, and A<sup>2</sup><sub>1g</sub> vibrational modes, confirming the presence of Bi<sub>2</sub>Se<sub>3</sub>. High-resolution HAADF-STEM images show that the Bi<sub>2</sub>Se<sub>3</sub> is highly oriented in the (0001) crystallographic direction. The quintuple layers of Bi<sub>2</sub>Se<sub>3</sub> (Se-Bi-Se-Bi-Se) were observed in the [110] crystallographic direction. The Photodetectors were made using microfabrication techniques inside the cleanroom with Cr/Au contacts. The devices' channel lengths range from 4 to 12 µm. From the I-V curves, the photodetectors respond to the light with a spectral response of  $5.804 \times 10^{-8}$  A/W. The results show that the devices generally follow an Ohmic behavior, confirming a good contact formation. Some of the device's contacts show Schottky diode behavior. Results from the Arrhenius plot show that the device has two different charge transport mechanisms with an activation energy of 0.28 eV for the temperature in the range from 200 K to 350 K. At lower temperatures, from 10 K to 200 K, the activation energy of the dark conductivity is 0.4 meV.

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## Visualizing Energy Transport in Nanostructured Semiconductors

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Nanostructured Semiconductors are a playing an increasingly dominant role for nextgeneration light-harvesting and light-emitting applications. In these materials, quantum confinement effects allow for enhanced control over their optoelectronic properties while reduced processing temperatures provide routes to more flexible integration. However, the reduced dimensionality and increased disorder can significantly impact the spatial dynamics of the energy carriers within the material.[1]

To study these effects, we employ Transient Photoluminescence Microscopy techniques which allow for a direct visualization of the excited state transport with few-nanometer and sub-nanosecond resolution. In this talk, I will highlight some of our recent efforts using this technique, with an emphasis on perovskite semiconductors of varying compositions and dimensionality. I will start the talk by giving an overview of some of the surprising effects that can be observed in these materials, particularly regarding the relationship between lattice softness and the exciton transport properties and the remarkably efficient interlayer transport.[2,3,4,5]

In the last part of the talk, I will present our most recent efforts using interferometric scattering techniques to study perovskite semiconductors. The exceedingly high signal-to-noise-ratio that interferometric scattering provides allows not only for the direct imaging of charge carriers, but also for super-resolution imaging of lattice dynamics.

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#### **Quasi-2D Ruddlesden-Popper nanoparticle-based photodetectors**

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Perovskites are favorable materials for light harvesting, and photonic applications due to their unique optoelectronic properties. They exhibit high carrier mobility, long-range carrier diffusion, high photoluminescence quantum yield, and tunable bandgap energy [1]. Perovskites in their bulk form exhibit extraordinary optoelectronic properties due to chargecarrier confinement and their electronic band structure. These properties result in remarkable enhancement in the efficiencies of solar cells, photocatalysis, LEDs, and photodetection. Despite their exceptional optoelectronic properties, their commercial usage is challenging due to lower chemical stability in the moist environment [2]. Improved optoelectronic property with enhanced stability is achieved in 2D halide perovskites by alternating cations in the interlayer space. These 2D halide perovskites can be synthesized using wet chemical synthesis or exfoliation [3, 4]. 2D halide perovskites show layer-dependent bandgap resulting in tunable excitonic confinement. The synthesis conditions control the crystal phase and dimensionalities of perovskites. we studied the optoelectronic properties and photodetection performance of quasi-2D methylammonium lead bromide perovskites with three different morphologies nanoplatelets (NP), nanosheets (NS), and nanostripes (NSP). The structural and optical characterization reveals the different extent of confinement due to its morphology. NSP shows the best photodetection performance due to the weaker confinement effect. NSP exhibits the highest photoresponsivity, EQE, and detectivity of 183 mA W<sup>-1</sup>, 56 %, and 2.9 x  $10^{11}$  Jones respectively. It also shows the fastest photoresponse with a rise time of 3.4 ms and a fall time of 4.3 ms compared to NP and NS. Our study will contribute to the development of an affordable, high-performance photodetector based on quasi-2D perovskites.

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## Luminescent, Semiconductor Nanoparticle-Loaded Polymer Microbeads – Comparing Particle Architectures

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Luminescent polymer microparticles (PMPs) are applied in various (bio)analytical and diagnostic processes.[1] The staining of these beads is important for the realization of optically distinguishable barcodes that can be read out, e.g., by a flow cytometer or fluorescence microscope. Typically, luminescent semiconductor nanoparticles (NPs) absorb in a broad wavelength range and show narrow emission bands, which enables simultaneous excitation of differently colored luminophores and facilitates a spectral discrimination.[1] This makes them ideal candidates for this purpose and encouraged us to explore and develop a simple, effective approach to luminescent semiconductor NP encoding of polystyrene PMPs and identify suitable synthesis conditions.[2]

Until now, mainly semiconductor quantum dots (QDs) have been used for the synthesis of luminescent PMPs, although NPs with different shapes could introduce beneficial new features. Aiming for the application of our developed procedure to non-spherical NPs, we systematically investigated the luminescence properties of the resulting NP-stained beads using fluorescence and integrating sphere spectroscopy as well as fluorescence and electron microscopy. These studies showed that the suitability of semiconductor NPs for the synthesis of luminescent PMPs depends not only on their shape, but also heavily on their surface chemistry.[3] The successful incorporation of nonspherical NPs opens the path to include even more NPs, and the results can help to deduce future applications for the beads which best suit their specific properties.

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## Effect of non-local theory on precise investigation of heat transport in semiconductor nanostructures using non-Fourier macroscopic models <u>Z. Shomali</u><sup>1</sup>

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Investigation of heat transport in micro/nanoscale semiconductor structures owing to their application especially in transistor technology, is a matter of interest. There exist atomistic and phenomenological macroscopic methods for heat transport study in semiconductor nanodevices. The atomistic models are more complicated, computationally expensive and simultaneously very accurate. Meanwhile, the macroscopic heat transfer models in support of less computational cost and acceptable but not very precise results, are introduced. The Dual Phase Lag (DPL) model presenting two phase lags of  $\tau_T$  and  $\tau_q$ , is one of the popular macroscopic schemes. It is obtained that using the DPL model for studying the temperature and heat flux behavior through the nanostructures, results in data which are almost near to that of the atomistic phonon Boltzmann equation (PBE). The present study tries to justify why DPL results are not very accurate and introduces the non-locality as a solution. The studied case is a silicon MOSFET. It is obtained that implementing the non-locality in heat flux is "the missing piece of the puzzle". While the conventional DPL presents not perfect but almost good results for high Knudsen number systems, including the non-locality makes the results, also for High Kn numbers, very close to that of the PBE data. The newly non-dimensional parameter y, presenting the strength of the nonlocality, is utilized through the nonlocal DPL modeling. The factor y is found to have a linear relationship with Knudsen (Kn) number, being 3.5 for Kn=10 and 0.035 for Kn=0.1. Hence, it is obtained that intruding y is critical for obtaining accurate temperature and heat flux distributions that are very close to the practical results of the Phonon Boltzmann equation [1].

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## Mapping the optical excitations with electron beams

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Van der Waals materials have enabled an exquisite platform for exploring light-matter interactions at the nanoscale. Various forms of van der Waals materials have enabled the observation of strong-coupling effects, in the form of exciton-polaritons, in either a self-hybridized form or in combination with photonic cavities. Here, I will elaborate on the interaction between free electrons and thin films of van der Waals materials, and will show how electron beams can probe self-hybridized exciton-polaritons in transition metal dichalcogenide thin films [1], and describe through a sequential cathodoluminescence spectroscopy technique the formation of a coherent cathodoluminescence radiation from exciton polaritons as well as their decoherence time scale [2]. I will also discuss how exciton-plasmon interactions can be leveraged to control the band structure of a plasmonic crystal [3]. In addition, the formation of exciton polaritons in perovskites [4], hyperbolic exciton polaritons in Bi<sub>2</sub>Se<sub>3</sub> [5], and hyperbolic plasmon-polaritons in borophene films [6] will be discussed and explored with electron beams.

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#### Solvation Shifts the Band-Edge Position of Colloidal Quantum Dots by nearly 1 eV

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The optoelectronic properties of colloidal quantum dots (cQDs) depend critically on the absolute energy of the conduction and valence band edges. It is wellknown these band-edge energies are sensitive to the ligands on the cQD surface, but it is much less clear how they depend on other experimental conditions, like solvation. Here we experimentally determine the band-edge positions of thin films of PbS and ZnO cQDs via spectroelectrochemical measurements. To achieve this, we first carefully evaluate and optimize the



Figure 1. Representation of a PbS cQD solvated the different solvent by molecules tested in this study (left). Conduction and valence band energies as a function of the Lewis basicity of the solvent surrounding the cQD. as determined by spectroelectrochemistry (right).

electrochemical injection of electrons and holes into PbS cQDs. This results in electrochemically fully reversible electron injection with >8 electrons per PbS cQDs, allowing the quantitative determination of the conduction band energy for PbS cQDs with various diameters and surface compositions. Surprisingly we find that the band edge energies shift by nearly 1 eV in the presence of different solvents, a result that also holds true for ZnO cQDs. Complexation and partial charge transfer between solvent and surface ions are responsible

for this large effect of the solvent on the band edge energy. The trend in the energy shift matches the results of density functional theory calculations in explicit solvents and scales with the energy of complexation between surface cations and solvents. As a first approximation, the solvent Lewis basicity can be used as a good descriptor to predict the shift of the conduction and valence band edges of solvated cQDs.

#### Advanced nanomaterials for the short-wave infrared

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There is a growing interest in the exploitation of the short-wave infrared (SWIR), which refers to the wavelength band of light between 900 nm and 2500 nm. Luminophores that emit in the SWIR are used in various areas of telecommunications, photovoltaics, security systems (night vision), and in biomedicine. In particular for biomedical applications, in vivo imaging in the SWIR range is highly promising because light scattering, absorption, and autofluorescence of tissue are strongly reduced compared to the visible (400-700 nm) and NIR (~700-900 nm). Full exploitation of SWIR photoluminescence (PL) imaging (PLI) is currently hampered by i.) a lack of suitable advanced nanomaterials with a high PL quantum yield (PL QY) and a high brightness, that can be used safely in vivo and ii.) a lack of quantitative and reliable data on the optical properties of many SWIR emitters.[1] Promising nanomaterials for the SWIR are atomically precise gold nanoclusters (AuNCs) and heavy metal-free Ag<sub>2</sub>S quantum dots (QDs). Thereby the optoelectronic properties of these nanomaterials can be modulated either by the variation of the surface ligand or by incorporating other elements like zinc into their crystal structure. Aiming for the development of SWIR advanced nanomaterials with optimum performance, we have dived deeper into the photophysical processes occurring in these nanomaterials, thereby exploring in depth how the environment, surface ligand composition, and the incorporation of transition metals influence the optical properties of AuNCs and Ag<sub>2</sub>S QDs. We observed a strong enhancement of the SWIR emission of AuNCs upon exposure to different local environments (in solution, polymer, and in the solid state). Addition of metal ions such as Zn<sup>2+</sup> to Ag<sub>2</sub>S based

NPs led to a strong PL enhancement, yielding PL quantum yields of about 10% and thus making them highly suitable for non-invasive deep imaging of vascular networks and 3D fluid flow mapping.

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#### Ultrafast hot carrier cooling enabled van der Waals

#### photodetectors at telecom wavelengths

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Photodetectors as significant components for on-chip optoelectronics play vital roles in modern imaging, sensing, and communication systems. Especially, photodetectors operating at telecom bands are highly preferred due to the low-loss transmission and the availability of optical gain. Two-dimensional (2D) materials with bond-free van der Waals (vdW) structures possess relatively mobility intrinsically picosecond large carrier and response time. demonstrating great potential for the next generation of ultra-thin photodetectors. However, due to the limited bandgap, the current 2D semiconductor-based-photodetectors for telecom C-band either rely on an integrated silicon waveguide or suffer from chemical instability. While in pursuit of broad photoresponse to use 2D semimetal, high dark currents would influence the performance.

Here we demonstrate a WS<sub>2</sub>/graphene heterostructure photodetector operating at 1560 nm with picosecond response speed and low dark current enabled by ultrafast hot carrier cooling. The vdW heterostructure ensures a highly efficient hot carrier injection from graphene to WS<sub>2</sub>, which frees it from waveguide integration. Power and temperature dependence indicate that the injected hot carriers preserve a cooling mechanism similar to that in pure graphene, inducing a response time of the photodetector down to 3 picoseconds. The dark current in our device is 5 orders of magnitude lower than a pure graphene-based photodetector and it can be further decreased by an optimized vertical WS<sub>2</sub>/graphene/WSe<sub>2</sub> device configuration with the same detection mechanism. The integration of 2D semiconductor and semimetal combines the merits of respective components and supports a simultaneously enhanced photodetector performance for integrated photonic circuits.

### **Abstracts of Posters**

(in alphabetical order)

#### Plasmonically Enhanced Solar Water Splitting with TiO<sub>2</sub>/Au/Pt Nanoparticles in PDMS Sponges

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Hydrogen (H<sub>2</sub>) generated out of renewable energy sources such as solar energy is an attractive alternative to the commonly burned fossil fuels. Indirect conversion methods such as electrolysis have rather low efficiencies. Utilizing the photocatalyst titanium dioxide (TiO<sub>2</sub>), direct energy conversion becomes possible.

With the excitation of electron-hole pairs by photo-absorption,  $TiO_2$  can drive the redox reaction involved in water splitting at the photocatalyst-water interface. Caused by its large bandgap of 3.2 eV,  $TiO_2$  can only absorb photons in the UV-regime. To sensitize the photocatalyst to frequency regions with higher intensities of the sun, i.e. the visible light regime, metallic nanoparticles (NPs) can be involved.

Under illumination, the electron gas of metallic NPs such as gold (Au) NPs oscillates with the incoming electric field. Its resonance, called localized surface plasmon resonance (LSPR), can be excited and decays into hot electrons that can be transferred onto the  $TiO_2$  NP and enhance the amount of reduction reactions at the photocatalysts' surface.

A novel method to increase absorption and maximize utilization of the incoming light is the implementation of NPs inside 3-dimensional (3D) polydimethylsiloxane (PDMS) sponges [1]. These PDMS structures offer a large surface for NP growth, leading to significantly higher absorption than in 2D NP arrangements.

Platinum (Pt) NPs can act as an efficient electron acceptor, reducing electron-hole recombination rates and thus enhancing the amount of  $H_2$  evolution reactions [2]. Based on these considerations, a new system consisting of TiO<sub>2</sub>, Au and Pt NPs incorporated in 3D PDMS sponges is under investigation.

A first gas sensor calibration has been performed to quantify the amount of H<sub>2</sub> produced. Such a measurement setup will allow further investigations on H<sub>2</sub> generation efficiencies of different NP systems in PDMS sponges.

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#### Using scattering microscopy to characterize semiconductor materials

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Microscopy techniques play a pivotal role in many scientific disciplines by enabling the visualization and tracking of materials at microscopic scales. Among the most used microscopy techniques is fluorescent microscopy, due to its high resolution and strong contrast[1]. However, its reliance on photoluminescence and high excitation powers imposes limitations, restricting its applicability. In contrast, scattering microscopy operates on a different principle, relying on the relative difference in refractive index between a sample and its substrate to achieve high resolution and contrast. This unique approach allows scattering microscopy to deliver sharp images with robust contrast across a wide range of materials, regardless of their fluorescence properties.[2] Moreover, the minimal excitation power required for imaging reduces photodamage and enables the tracking of material properties over both short and extended timescales. These benefits make scattering a perfect contrast mechanism for transient microscopy.[3]

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#### Long-range self-hybridized exciton polaritons in two-dimensional Ruddlesden-Popper perovskites <u>Maximilian Black<sup>1</sup></u>, Mehdi Asadi<sup>2</sup>, Parsa Darman<sup>2</sup>, Sezer Seçkin<sup>3</sup>, Finja Schillmöller<sup>1</sup>, Tobias A.F. König<sup>3</sup>, Sara Darbari<sup>2</sup>, Nahid Talebi<sup>1</sup>

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Ruddlesden-Popper perovskites combine the widely known perovskite properties of excellent photoluminescence efficiency and high synthetic versatility with a crystal structure of stacked quantum wells. This structure leads to two-dimensional quantum-confinement, resulting in the bulk crystal exhibiting features usually known for semiconductor mono- or bilayers, such as further enhanced exciton binding energies and



exceptionally high quantum yield<sup>1</sup>. These features make them exciting platforms for the study of exciton-polaritons, mixed states of excitons and localized photons.

In this work<sup>2</sup>, we present proof of the formation of long-range propagating excitonpolaritons in the cavity made of the crystal itself, a phenomenon called selfhybridization<sup>3,4</sup>. Spatially and angle-resolved optical spectroscopy shows splitting of the excitonic resonance and polaritonic bending of the dispersion of the Fabry-Pérot modes, while photoluminescence spectroscopy unveils multiple polariton branches with thickness dependent energies. Strikingly, local optical excitation below the exciton energy results in the coupling of light to in-plane polaritonic modes and transfer to lower-energy polaritons. leading to detectable energy а signal. The exciton-polaritons exhibit directed photoluminescence long-range propagation with high coupling efficiencies and low loss, as confirmed by finitedifference time-domain simulations. Thus, we demonstrate that mesoscopic 2D Ruddlesden-Popper perovskite flakes serve as an effective and straightforward system for exploring the rich physics of exciton-polaritons at room temperature.

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#### Exploring Low Dimensionality in Perovskite Materials

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Perovskite materials have gathered significant attention due to their remarkable optoelectronic properties and potential applications in various fields. This study explores the synthesis and characterization of perovskite materials with a particular emphasis on diverse dimensionalities, especially 1D wires and 2D sheets. Some synthetic methods offer control over the size and shape of perovskite nanostructures [1], facilitating a comprehensive exploration of their optical properties.

The 1D nature of perovskite nanowires can provide excellent electrical, optical, and physical properties, such as improved light trapping, lower defect density, longer photocarrier lifetime and better mechanical properties, and have been used for solar cells, photodetectors and LEDs, among others [3]. The key question then is understanding how excitation travels through the material and whether this behavior differs from that in the bulk material solely due to the shape. We can directly visualize the spatial movement of energy carriers with sub-nanosecond and few-nanometer resolution by employing transient photoluminescence microscopy [2].

These studies provide crucial insights into the dynamic behavior of excitons and free charges within these materials and their relationship with the local morphology. The findings from this study not only deepen our understanding of perovskite nanomaterials but also pave the way for their use in advanced optoelectronic devices and applications.

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#### Visualizing the energy transport of Perovskite Quantum-Dot Networks

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Perovskite quantum-dot solids (pQDs) are explored as a promising candidate for next-generation photovoltaic, light-emission, and photodetection devices. Their charge transport characteristics are dominated by the quantum confinement effects of the QD and electronic coupling among the different nanocrystals. Recently, ligandfree QD assemblies have emerged as an alternative to colloidal QDs, since they can be directly grown into porous matrices with optical quality and charge transport properties. Studies have shown that transport in these matrices decreases with decreasing precursor concentration, leading to poor interconnectivity between QDs [1]. However, these studies have been performed using macroscopic photoluminescence and absorption spectroscopy [2], and a microscopic picture of carrier transport through these complex matrices is lacking. The visualization of the energy transport using transient photoluminescence microscopy is key to improve our understanding of the carrier transport through the device [3]. Here, we present Transient Microscopy studies that directly visualize carrier transport with sub-ns and few nanometers resolution. This experiment allows us to study carrier diffusion by measuring its photoluminescence after laser beam irradiation. Our experiments show that the diffusion coefficient decreases with the perovskite concentration. Importantly, diffusion maps are consistently asymmetric. Our results are a strong indication for the formation of percolation paths in these samples. We will discuss theoretical modelling that can capture the complex spatiotemporal dynamics of carriers in these materials and provide design rules for optimized performance.

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#### Enhanced Wide-Field Transient Photoluminescence Microscopy Using Fast-Gated ICCD for Carrier Transport Studies

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Transient photoluminescence microscopy techniques are essential for investigating carrier transport in semiconductor materials, offering sub-nanosecond temporal resolution and nanometre spatial resolution by detecting changes in the spatial distribution of a diffraction limited population of carriers via radiative decay measurements<sup>1</sup>. However conventional time-resolved photoluminescence (TRPL) setups typically employ discrete detectors such as avalanche photodiodes or photomultiplier tubes, which measure transient PL at a single location on the sample. This method requires multiple measurements at different positions to monitor carrier diffusion comprehensively making it time-consuming and potentially inaccurate if too few locations are sampled or if prolonged scanning leads to sample degradation. To overcome these limitations, a modern wide-field transient PL imaging method utilizing a fast-gated intensified charged coupled device (ICCD) presents significant advantages. This technique employs a megapixel intensified camera to replace the point detector enabling parallelized measurements across a wide observation field<sup>2</sup>.

The ICCD's high temporal-spatial resolution over a substantial field of view and its fast-gating capability, facilitates the construction of high signal-to-noise ratio images for various delay times. This parallelized approach significantly reduces measurement time and enhances the exploration of carrier diffusion under different conditions and minimizes the risk of sample degradation due to the reduced need for repeated scanning. The integration of ICCD technology into wide-field transient microscopy represents a substantial advancement, providing improved spatial-temporal resolution, faster measurement times and a broader spectral response, making it a powerful tool for investigating the dynamics of optoelectronic materials.

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#### Time-resolved photocurrent spectroscopy on gold nanorods

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In an increasingly fast-moving world, in which the internet reaches your doorstep via optical fiber, faster optical switches are becoming more and more important. They convert the optical signal from the optical fiber into an electrical signal that is processed by the computer at your desk. This makes it possible, for example, to search for the latest literature on gold nanorods from an office chair.

These could prove to be a promising material for an optical switch because their electrons are excited very quickly by plasmonics and because they have a negative photoelectric effect. This is indispensable in optical switches, as otherwise the incoming optical signals could not be recognized.

Different ligands on the nanorods and different wavelengths are used in attempt to enhance the photoelectric effect and, above all, to shorten the times required by the systems to reach the value of the photocurrent from the value of the dark current or vice versa. This is referred to as the rise time at the beginning of the light irradiation and, similarly, the fall time at the end. In each case, the time required to rise/fall from 10 % to 90 % of the final value is calculated. For fast optical switches, it is important to keep these times as short as possible. With a negative photoelectric effect, such as that of the gold nanorods, this means that the current level decreases when the laser is switched on and increases again when it is switched off.

The time required for the samples to reach the photocurrent or the dark current again is in the range of several seconds and is therefore too long for it to make sense to incorporate the nanorods directly into optical switches.

The potential for using gold nanorods in optical switches is considerable, even if the right system has yet to be found.

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#### Boosting the magnetic response of a composite nanostructure in the optical region with a Fano resonance

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At optical frequencies, the magnetic response of all materials to light is far weaker than their electric response, as the relative magnetic permeability of all natural materials drops of to 1 at higher frequencies (Landau-Lifshitz limit). However, artificial magnetism can be achieved by utilizing plasmonic nanostructures that guide the plasmonic current along a circular loop to induce a magnetic moment. A split-ring resonator (SRR) is a commonly used structure to achieve artificial magnetism. This structure consists of a nanoring with a gap. SRRs and their magnetic resonance have already been investigated for many applications, such as metamaterials, sensing, and super-chiral near fields. However, saturation effects limit the magnetic resonance frequency of a SRR to the THz and infrared regime [1]. We propose a modified SRR geometry with two additional gaps to shift the magnetic resonance towards higher frequencies. This proposed structure and its properties are investigated with numerical simulations as well as experimental fabrication - using electron beam lithography and helium-ion milling - and measurement by dark-field spectroscopy. Additionally, we demonstrate that the magnetic response of the nanostructure can be improved by adding a nanorod below the central element of the SRR. Two parallel nanorods have another magnetic resonance that is excited through a coupling to the magnetic resonance of the SRR. This coupling between the modes leads to an interference phenomenon called Fano resonance, which changes the scattering behaviour of the nanostructure. The excitation of the additional magnetic mode contributes to the magnetic response of the nanostructure, increasing it by 70%. Such an increase of the magnetic response may help with the performance of applications of the SRR at higher frequencies, for example metamaterials, perfect absorbers, magnetic mirrors, or Huygens metasurfaces [2].



Figure 1. a) Scheme showing the SRR with additional gaps. b) Scheme showing the extended SRR with the additional nanorod below the central element

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#### Ligand-Induced Structural Modulation on Nickel Redox States in 2D Metal-Organic Frameworks

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Two-dimensional metal-organic frameworks (2D MOFs) attract considerable attention because of their versatile properties and potential applications in single-atom catalysis, high-density storage media or molecular electronics and spintronics. Here, we investigate the intrinsic magnetic and electronic properties of a single-layer MOF on graphene, taking advantage of the weak interaction between the MOF and the graphene substrate. Through a combination of spectroscopic characterization and theoretical modeling, we explore how the coordination environment influences the magnetic cores and electronic behavior of this 2D material. Notably, we observe two distinct coordination environments of transition metal (TM) cores within the 2D MOF and clarify how structural modulations in the ligand field determine the hybridization between the Ni 3d states and the  $\pi$ -symmetric molecular orbitals of 7,7,8,8tetracyanoquinodimethane (TCNQ) ligands, leading to the coexistence of two redox states of the metal centers in the framework. Furthermore, we examine the transition from free-standing MOF on nearly inert graphene to metal-supported frameworks synthesized on Au(111) and Ag(100) substrates, elucidating the impact of substrate interactions on the electronic properties. Our findings contribute to advancing the general understanding of MOFs and offer insights into the development of functional materials with tailored magnetic and electronic characteristics.

#### Wet synthesis of 3D confined materials for plasmonic sensing and catalysis

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The phenomenon of plasmon excitation on the surface of metal nanostructures (NSs) becomes a starting point for the field of plasmon catalysis and sensing, which seeks to maximize conversion of light to a wide range of chemical reactions or enhancement of analytical signal. In order to maximize the interface between molecule of interest and intense local electric field ( $|E|^2$ ), quasi-3D plasmonic volumes or pores with features in the same order as the excitation wavelength could be synthesized. Extended arrays of pores in three dimensions will enhance both local and long-range plasmon coupling effects.

To prepare these 3D plasmonic confined materials, recently we developed an inexpensive and scalable wet chemistry method. This method includes deposition of mesoporous metals (e.g., Au, Ag, Cu) on conductive surfaces by co-depositing block copolymer micelles (BCM) with metal using a simple electrochemical setup [1,2]. The size of the mesopores can be tuned from 5 to 40 nm in diameter depending on the diameter of the BCM, and the resulting subwavelength pores interact strongly with light to enable sensing and/or catalysis [3,4].

These porous plasmonic NSs demonstrated an advantageous application for surface-enhanced Raman spectroscopy (SERS) [3] and organic transformation [4].

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#### Template Mediated Formation of Colloidal 2D SnTe Nanosheets and the Role of the Ligands

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As a IV-VI narrow bandgap semiconductor (0.18 eV, bulk), SnTe exhibits an intrinsically high charge carrier concentration, which results in a relatively low Seebeck coefficient, <sup>[1, 2]</sup> but optimization of the material through doping and alloying offers great promise for thermoelectric applications of this material. SnTe has also gained significant interest due to its exciting properties as a topological crystalline insulator, IR detection and radiation receivers material, as well as photovoltaic absorber. So far, attempts to obtain solution-based SnTe nanocrystals (NCs) mainly yielded zero-dimensional (0D) or one-dimensional (1D) nanostructures. Recently we reported a synthesis protocol for two-dimensional (2D) colloidal SnTe nanostructures. Now, we disclose the important role of ligands in the colloidal synthesis process information of the 2D morphology and the observed faceting of nanocrystals. Since SnTe has a cubic crystal structure and octahedral coordination geometry, the formation of anisotropic shapes has to be conducted by molecular templates. These templates are well-organized domains consisting of the cation and a specific combination of ligands/counterions. When the tellurium precursor is injected into the reaction mixture, the tin/halogen arrangement of the template is replaced by the Sn-Te bond, and a bilayer oleic acid shell is formed simultaneously. These results emphasize the importance of co-ligands in the synthesis and explain the mechanism behind 2D SnTe nanostructure formation, providing a basis for stable, tunable lowdimensional nanomaterials.



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### Simulation of Charge-Carrier Transport in Cadmium Sulfide Nanowires

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Theoretical simulations form the backbone of experiments and help to confirm physical models, find material properties, and also provide more detail in results such as spatial resolution. Here we report on a numerical finite element simulation of single electrically contacted cadmium sulphide (CdS) nanowires using COMSOL Multiphysics® software. The focus of the simulation is on the surface potential, the band alignment and the current-voltage behavior. The results are compared with experimental results obtained by local photocurrent microscopy and Kelvin probe force microscopy on single wet-chemically synthesized CdS nanowires. This comparison gives us a better understanding of the underlying physics and provides material parameters that are difficult to obtain by experiments alone.

We show that simulations based on the drift-diffusion approach including trap-assisted charge-carrier recombination at the surface, local photo excitation and ohmic metal contacts on the surface, is able to provide comparable results and new insights, for example, into the type of recombination or the exact location of the electrons and holes. We can also see how the system behaves under extreme conditions, such as high applied voltages or temperatures.

# Ligand-dependent charge carrier dynamics in perovskite nanocrystal LEDs with polar electron transport layer

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Perovskite nanocrystals (NCs) have gained significant interest in the research community for light-emitting applications owing to their exceptional optical properties. Having a highly dynamic and unstable surface, passivation of these surfaces with appropriate ligands becomes crucial<sup>1</sup>. Despite advances in stability and optics, the electrical impact of these ligands in device is often overlooked. In addition, it is well established in the literature that polar organic molecules such as TPBi exhibit giant surface potential (GSP) due to intrinsic polarization which can alter carrier dynamics in organic optoelectronic devices<sup>2</sup>. Given that TPBi is extensively used as an electron transport layer (ETL) in perovskite light emitting diode (PeLED) stacks, the influence of its intrinsic polarization on perovskite NCs has not been studied so far.

In this study, we investigate cubic CsPbBr<sub>3</sub> nanocrystals passivated with oleyl amine/oleic acid (OLA/OA) and ligand-exchanged with didodecyldimethylammonium bromide (DDABr) respectively. The carrier dynamics of these systems is explored by considering a PeLED device. A significant increase in external quantum efficiency (EQE) is observed with polar ETL, due to enhanced charge injection by the ETL's intrinsic polarization. Ultraviolent photoelectron spectroscopy (UPS) indicates a higher GSP effect for ligand-exchanged particles. A unique voltage-dependent PL intensity quenching behaviour is observed in both systems where polar ETL suppresses the overall quenching. These results suggest that unlike organic devices, the effect of GSP in PeLEDs is greatly influenced by the ligand system; and it is essential to understand deeper the ligand interaction with the NC surface and its influence on the electronic properties.

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#### Fabrication and Characterization of Iron Titanate Thin Films as a Potential Tunnel Barrier for Magnetic Tunnel Junction (MTJ's)

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Spintronics addresses rising power dissipation in electronic circuits by offering advantages such as 0% standby leakage, low power consumption, unlimited durability, non-volatility, and compatibility with CMOS technology [1]. In this research work focuses on magnetic tunnel junctions (MTJs) in spintronics, investigating the barrier layer for efficient electron spin transfer, crucial for Magnetic Random Access Memory (MRAM). Iron titanate thin films have attracted research interest due to their potential applications in spintronic devices [2]. An application-oriented electrodeposition technique was used to prepare iron titanate thin films with varying electrolyte molarities [1,2]. XRD results reveals the amorphous behavior of Asdeposited thin films. Magnetic field (MF) annealing improved the structural and magnetic properties, the Fe2TiO4 phase was observed, confirming a spinel structure with increased crystallite size and strengthened phase as molarity increased. Magnetic analysis using a vibrating sample magnetometer (VSM) showed soft ferromagnetic behavior in annealed thin films, while the as deposited thin films show para-ferromagnetic mixed behavior. Asdeposited films had lower saturation magnetization compared to annealed films.

In conclusion,  $Fe_2TiO_4$  thin films fabricated via electrodeposition demonstrate significant potential for future spintronic devices specifically in the advancements of MRAM technology.

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#### Tailoring Quantum States in Coupled Cylindrical Quantum Dots through STIRAP

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In this study, we explore the principles of Stimulated Raman Adiabatic Passage (STIRAP) and its relevance in manipulating the quantum states of two coupled cylindrical quantum dots using modified Pöschl-Teller confinement potential in the axial direction and a parabolic potential in the radial direction through the density matrix formalism. We simulate a connected three-level system made up of two Ga<sub>1-</sub> <sub>x</sub>Al<sub>x</sub>As quantum dots (QDs) in a GaAs environment. Careful manipulation of aluminum (Al) concentration within the QDs has led to the creation of a three-level energy structure within the system. Employing the theoretical framework of density matrix formalism, we quantitatively determine the probability distributions characterizing the presence of an electron within the bound quantum dots across the three discrete states. Furthermore, the potential utilization of STIRAP for the purpose of manipulating quantum states within the two QDs is also examined and discussed.

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# Exciton binding energy and interband absorption in a cylindrical quantum dot GaN/InxGa1-xN

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Quantum dots represent a particularly intriguing class of materials due to their unique crystalline structure, characterized by the emergence of a substantial internal piezoelectric field, even at low indium concentrations. This distinctive feature renders them versatile for a wide range of applications, including light-emitting diodes spanning from red to ultraviolet wavelengths, solar panels, microcontrollers, and energy generation technologies. This research delves into the exploration of exciton states within cylindrical Gan/In, Ga<sub>1,</sub>N quantum dots (QDs). To effectively model the confinement potential of such QDs, the modified Pöschl-Teller potential is employed in the axial direction, while for the radial direction parabolic potential is used. The study initially focuses on assessing the dependence of critical parameters. This includes the wave function, ground, and first excited state energies, as well as binding energies. These dependencies are examined regarding with the geometric characteristics of the quantum dot and the concentration of indium within the material. Of particular interest are the observed effects of varying indium concentrations, which have a profound impact on the internal piezoelectric field, influencing the spatial separation of electron-hole pairs and modulating the band gap curvature. Subsequently, our investigation extends to the analysis of absorption processes, specifically the interband absorption and the creation of the electron hole pair. We scrutinize the intricate relationships between these absorption processes, the geometric properties of the quantum dots, and the indium concentration. In addition, the selection rules have been revealed for the corresponding quantum transitions. In summary, this study provides valuable insights into the excitonic properties of cylindrical Gan/In, Ga1-r, N quantum dot considering taking into account piezoelectric effects arising due to the indium concentrations.

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#### Development and Optimization of RoHS-Compliant In(As,P) Colloidal Quantum Dots for Enhanced Optoelectronic Devices

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In(As,P) colloidal quantum dots (QDs) with a band-edge absorption feature at 1300 nm are suitable candidates for RoHS-compliant optoelectronic applications due to their synthesis by employing non-toxic, commercially available precursors. These QDs require post-processing through ligand exchange protocols to stabilize the colloids as inks for device integration. Specifically, short-chain ligands aid in passivating strap states found in III-V QDs.

To stabilize colloidal QDs, a 2-phase liquid-liquid extraction approach was employed, involving n-butylamine and/or 3-mercapto-1,2-propanediol (MPD) as extracting agents, and ZnBr<sub>2</sub> as a passivating component. This method effectively replaces the native long-chain ligands with short-chain molecules, resulting in the phase transfer of QDs to a polar solvent, and is crucial for enhancing the charge-carrier mobility in QD films used as absorber layer in infrared photodetectors.

Significant passivation of trap states after incorporation of ZnBr<sub>2</sub> was confirmed by spectrofluorimetry, exhibiting a considerably enhanced emission intensity relative to the samples not treated by ZnBr<sub>2</sub>. Post-processed QDs are integrated into field-effect transistors (FETs), exhibiting an electron mobility in the order of 10<sup>-3</sup> and 10<sup>-2</sup> cm<sup>2</sup>.v<sup>-1</sup>.sec<sup>-1</sup> for DMF- and FA-based inks respectively.

ZnO nanocrystals, Poly-TPD, and MoO<sub>3</sub> are utilized as the electron transport layer (ETL), hole transport layer (HTL), and electron blocking layer, respectively. The quantum dot photodiode (QDPD) stack achieves an external quantum efficiency (EQE) of 19% at -2 V, which is significantly higher than previous SWIR-sensitive QDPD stacks using the reference ligand exchange protocol<sup>1</sup>.

Our findings highlight the potential of non-hazardous InAs QDs with different ink formulations as photo-active layers for short-wave infrared (SWIR) sensors and imagers. These results are promising due to the non-hazardous methods that avoid TMS or hydride-based chemicals.

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## Controlling the photofunctional properties of heterostructured Cu<sub>2</sub>O/Au nanoparticles by the arrangement of gold

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As appealing photofunctional materials, heterostructured semiconductor/noble metal nanoparticles are considered to be among the most promising candidates for conversion, sustainable energy especially in solar-driven photocatalysis. Semiconductor nanoparticles integrated with metal components serve two purposes by increasing the absorption range from UV to visible and improving the separation of the photogenerated charge carriers. We have published a report on the wet-chemical synthesis of Cu<sub>2</sub>O/Au multicomponent nanoparticles in two different configurations: (i) the surface of octahedral-shaped Cu<sub>2</sub>O nanoparticles was decorated with gold nanograins, and (ii) single gold nanorods were embedded into Cu<sub>2</sub>O nanooctahedra. The size, shape, and composition were identical for both model systems, allowing us to unveil how the presence and position of gold influence the optical and photocatalytic properties of the pristine Cu<sub>2</sub>O nanooctahedra. Charge carriers were excited solely in the Cu<sub>2</sub>O compartment by an excitation source being off-resonance with the LSPR of gold, enabling us to focus on understanding their separation process. Using a low-powered illumination source, we found the pristine Cu<sub>2</sub>O nanooctahedra to be inactive in photocatalytic dye degradation, while the heterostructured Cu<sub>2</sub>O/Au nanoparticles showed great performance. The designed model system allowed the utilization of a low-powered illumination source to drive a photocatalytic reaction, thus providing a platform for the sustainable treatment of pollutants. [1]

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# Tuning the surface properties of CuO films using the precursor aging approach for enhanced photoelectrocatalytic reactions

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#### Abstract

The surface properties of semiconductors significantly influence their photoelectrocatalytic efficiency in water splitting. This research presents a precursor aging method for tuning the surface properties of CuO films, for enhanced catalytic response. A precursor solution made using copper acetate, PEG 400, and diethanolamine, and age for 1, 40, 80, 120, 150, 180, and 250 days were used to fabricate CuO photocathodes via the dip-coating method. The films fabricated using the 1-day-old precursor reveal compact and homogeneous nanoparticles. The film's surface eventually got tuned to yield highly porous and rougher surfaces after aging the precursors for 180-250 days. The bandgap of the films decreases by 9% after 180-250 days of precursor aging. Photocathodes prepared using the 180-day-old precursor produce the optimum photocurrent density of 1.6 mA/cm2 at 0.35 V vs RHE, representing a 196% increase relative to the films fabricated using the 1-dayold solution. In addition, the photocathodes produce an anodic onset potential shift of 260 mV. This improved photoelectrocatalytic response is due to the porous morphology of the films, which provides a larger surface area that enhances light absorption, increases active sites for catalytic reactions, and reduces resistance to charge transfer at the photocathode-electrolyte interface.

#### A Comparative study of pressure effect on the structural, electronic and optical properties of LaXO<sub>3</sub> (X = Al, In, Ga) for Optoelectronic Applications

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The perovskite materials  $LaXO_3$  (X = AI, In, Ga) are investigated for their structural, electronic, elastic, mechanical, and optical properties using a first-principles study based on density functional theory (DFT) with the hybrid functional (HSE) method. We used HSE based upon WIEN2k code. The compressive investigation under the external static isotropic pressure (P= 0 to 80GaP), phase stability, band structure and their important impact on the optical response of LaAlO<sub>3</sub>, LaTiO<sub>3</sub> and LaGaO<sub>3</sub>. Structure stability under suitable pressure conditions is inspected under the Goldschmidt tolerance factor and elastic stability criterion. The valuable effect of pressure, on the electronic response of band gap tuning LaAlO<sub>3</sub>, LaInO<sub>3</sub> and LaGaO<sub>3</sub> continually enhanced and showed their indirect nature. Under main desperation physical parameters of perovskite materials are well explained the response of TDOS, and PDOS contour plots have been well understood for the full description of the band gap. Additionally, to verify the authenticity optical response of the title perovskite materials are estimated analysis the Kramer-Kroning approach. The optical tunings under the effect of pressure which are good candidates in practical optoelectronic applications are extensively used and interpreted by the calculation of the dielectric function.

#### Surface Lattice Resonances in Plasmonic Gold Nanocone Arrays

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Plasmonic excitations in isolated noble metal nanoparticles suffer from strong damping of the induced charge density oscillations. In addition, the plasmonic resonances are mainly tailored by the preparation of different, predetermined particle geometries, which can be cumbersome during the fabrication process. These limitations can be tackled by arranging single plasmonic antennas of one particular geometry in regular lattices. By doing so, a coupling between the isolated particles and the lattice is achieved by the excitation of surface lattice resonances (SLRs). The coupling is due to phase matching between the light radiated by all individual particles and the excitation light. This strongly modifies the spectral response and reduces the damping of the entire system. Further interesting optical responses, such as tailoring of the emission angle, fluorescence beaming, etc. can be realized [1, 2]. In this contribution, SLRs excited in plasmonic gold nanocone lattices with square symmetry are investigated in terms of the coupling strength between the single emitters. A distinction is made between in-plane and out-of-plane excitations with respect to the substrate surface, where for the latter an increased light-matter coupling is expected due to the coupling to more nearest-neighboring particles. Cone-shaped particles were specifically chosen as they support orthogonal in-plane and out-of-plane single particle resonances. The role of the substrate, introducing a refractive index mismatch compared to the medium, is investigated in terms of the stability of the SLRs with the application in sensing studies in mind. The formation of SLRs is investigated in scattering and extinction measurements (cf. Fig. 1), visualizing the energy-momentum space for a determination of the coupling strengths.



Fig. 1: Simulated dispersion of the extinction of a square gold nanocone array with a = 500 nm lattice period as a function of the excitation angle. Ppolarized light and a homogeneous medium are used.

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#### An investigation into the potential of lanthanum oxide halides as gate dielectric materials in transistors

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The transistor industry is continually focused on improving materials to achieve the highest possible efficiency. Two-dimensional (2D) materials, known for their superior properties, are now seen as more promising than traditional silicon and its oxides. A novel family of compounds, lanthanum oxide halides (LaOX), has been theoretically predicted to act as 2D van der Waals dielectrics, with some members exhibiting highκ values[1]. In this study, we synthesized and analyzed several LaOX compounds, including LaOI, LaOBr, and LaOCI, as potential gating materials for 2D FETs. The synthesis was performed by flux growth in an open corundum crucible, producing LaOX crystals with typical sizes of up to several millimeters. We characterized these materials using SEM-EDS, XPS, and Raman spectroscopy, which confirmed their expected compositions. To evaluate their electrical properties, we transferred on prearranged Si/SiO<sub>2</sub> substrates thin flakes of mechanically exfoliated LaOX onto graphene/MoS<sub>2</sub> channels, fabricating double-gate FETs. Using graphene allowed us to measure the out-of-plane static dielectric constants[2] for all three materials. Our results show a clear correlation between the relative permittivity and the type of halogen atom in the compound. Additionally, we observed variations in exfoliation efficiency, which could affect the practical application of these materials. In conclusion, this research highlights the promising potential of the LaOX family as dielectrics for next-generation FETs, particularly due to their tunable dielectric properties based on halogen content.

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# Plasmonic nanoantennas for boosting TMDC based photodetection

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In the last few decades, TMDC (transition metal dichalcogenide) semiconductors have become of great interest for photodetectors due to their outstanding optoelectronic properties. While there are many studies on their responsivity, our group is more interested in their temporal resolution, e.g. the application as 2D optical converters of optical fibers. However, since the bandwidth improvement of pure TMDC flakes seems to be limited [1], the work presented here is based on plasmonic enhancement of these materials.

By placing differently shaped plasmonic structures in the measured electrode channels, the aim is to improve both the absorption and the near-field around the flakes which is expected to lower the resistance and thus the current limitation of the devices so far [2]. To achieve this goal, different lithographic methods (e.g. optical/electron beam lithography) will be used and combined to exploit their individual advantages.

This combination of TMDCs and plasmonic nanoantenna's is expected to overcome the current limitations of pure TMDCs and may at some point even provide an alternative to silicon-based photodetectors.

The poster provides the device fabrication as well as the measurement setup and its underlying measurement principle.

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#### Engineering the Electronic and Spin Configuration in 2D Metal-Organic Frameworks through Transition Metal Core Selection

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The electronic and magnetic properties of metal-organic frameworks (MOFs) are to a great extent defined by the nature of the metal core and the coordinating organic ligand. For this reason, the present research employs a multi-technique approach, supported by theoretical calculations, to comprehensively study the local electronic structure of two-dimensional MOFs. The MOFs chosen for this study are composed by 1,2,4,5-tetracyanobenzene (TCNB) as the organic ligand and transition metals (TM) as metal cores, all deposited on an Ag(100) substrate.<sup>[1,2]</sup>

Low-energy electron diffraction experiments demonstrate that the MOFs form commensurate superstructures with long-range order. Angle-resolved photoemission spectroscopy is then employed to examine the evolution of the band structure of the MOFs. In comparison to the photoemission data of a monolayer of TCNB molecules self-assembled on silver, new energy-dispersive electronic states with hybrid character emerge upon MOF formation. These states arise from the interaction and overlap between the 3d states of the TM and the ligand  $\pi$  molecular orbitals. This interaction stabilizes specific electronic and spin configurations of the TM ion, as demonstrated by x-ray photoelectron spectroscopy and x-ray magnetic circular dichroism experiments.

The study includes three different TMs, namely Fe, Co and Ni. Despite the three MOFs manifesting equivalent geometrical ordering, the TMs display different energy level alignments in terms of their 3d states. As a result, the hybrid states are centered at different energies, and most importantly, different bandwidths are observed. We conclude that the TM selection is crucial in controlling the MOF properties, particularly as the strategic engineering of the orbital overlap governs the electronic and magnetic properties in the MOFs.

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#### Unveiling γ-Cul as a Promising Hole Transporting Material: A DFT Investigation for Enhanced Perovskite Solar Cells

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Perovskite solar cells (PSCs) are recognized for their high efficiency and potential for low-cost production. However, the use of organic Hole Transporting Materials (HTMs) in these cells poses challenges due to their high cost and tendency to degrade the perovskite layer over time, threatening the commercial viability of PSCs.

In this study, we employed first principles calculations based on Density Functional Theory (DFT), utilizing both the Generalized Gradient Approximation (GGA) and GGA + Hubbard correction, to evaluate the potential of  $\gamma$ -Cul as a cost-effective HTM.

Initial investigations involved a thorough geometry optimization to ensure structural stability, followed by an analysis of elastic and mechanical properties, which demonstrated the material's suitability for use in flexible PSCs [1].

The electronic and optical properties of  $\gamma$ -Cul were explored, revealing a low extinction coefficient and high refractive index across the infrared and visible spectra. Notably,  $\gamma$ -Cul demonstrated minimal reflectivity and absorption in key spectral regions, highlighting its potential to reduce optical losses in PSCs [1].

These findings position  $\gamma$ -Cul as a promising and economically viable HTM, offering significant advantages for the next generation of perovskite solar cells.

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## Charge Carrier Diffusion Diversity in Various Colloidally Synthesized MAPbBr3 Perovskite Morphologies

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In the field of optoelectronic applications, metal halide perovskites (MHPs) are gaining traction due to their tunable optical properties. [1,2] The process of colloidal Synthesis allows the creation of various MHP morphologies, each with its unique carrier properties and, consequently, distinct optical and transport behavior. Our study focused on three different Methylammonium lead tribromide perovskite (MAPbBr3) morphologies - nanoplatelets (NPLs), nanosheets (NSs), and nanostripes (NSTs). [3] By analyzing emission and absorption measurements using Elliott formalism, we revealed the layered structure of the NSs and NPLs, while the NSTs exhibited a bulk nature. [4] Additional measurements of carrier lifetimes provided valuable insights into the charge carrier types and recombination behaviors. To further our understanding, we employed a modified fluorescence imaging microscope (FLIM) for a time- and space-resolved measurement of carrier migration. Our findings revealed the highest carrier diffusivity in the bulk-like NSTs, followed by the layered NSs and a thin film of NPLs. These findings have potential applications in the development of optoelectronic devices with enhanced performance.

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#### Electrodeposited Zirconium Titanate Thin Films: Structural, Magnetic, and Dielectric Properties for Spintronic Applications

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Zirconium titanate (ZrTiO4) thin films have emerged as a cornerstone material in the advancement of spintronic devices, owing to their exceptional structural, magnetic, and dielectric properties [1,2]. This study harnesses a precise electrodeposition technique to fabricate ZrTiO4 thin films, meticulously varying the molarity of electrolytes from 0.01M to 0.05M. X-ray diffraction (XRD) analysis reveals a transition from amorphous behavior at 0.01M to the formation of phase-pure, orthorhombic ZrTiO4 at higher molarities, with a notable increase in crystallite size, indicative of enhanced phase stability. Vibrating Sample Magnetometer (VSM) measurements demonstrate a pronounced soft ferromagnetic behavior, with an impressive saturation magnetization peaking at 29 emu/cm<sup>3</sup> at 0.05M. Dielectric studies reveal a significant dielectric constant of 180 at log f=2 and a minimal tangent loss of 0.02 at 0.05M, showcasing superior dielectric performance. Cole-Cole plots further elucidate the dielectric properties, indicating dominant grain boundary resistance. The comprehensive analysis underscores the potential of ZrTiO4 thin films as pivotal components in next-generation spintronic devices, offering unparalleled structural integrity, magnetic provess, and dielectric efficiency [2].

These findings pave the way for the integration of ZrTiO4 thin films in high-performance, energy-efficient spintronic applications, marking a significant leap forward in material science and device engineering.

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#### Layered metal thio (seleno) phosphates for broadband optoelectronics

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A large number of promising two-dimensional (2D) semiconductor materials, represented by black phosphorus (0.3 eV), transition metal dichalcogenide (TMDCs) (<2 eV), and hexagonal boron nitride (6 eV), have been extensively studied in optoelectronic devices. However, the spectrum of large-band gap materials remains very narrow, limiting the application for broadband optoelectronic devices. The broad family of metal thio and selenophosphates with large tunable band gaps (1.5-3.5eV), which can be adjusted by varying the metal cation and the anion during the synthesis, can bridge the gap of intermediate band gaps (1.5-4 eV) between TMDCs to hBN. We present the synthesis and fabrication of high-performance broadband photodetector based on multilayered CulnP<sub>2</sub>Se<sub>6</sub> and CulnP<sub>2</sub>S<sub>6</sub>. Both samples were prepared by the CVT method. The samples were thoroughly characterized by in-depth microscopic (SEM, HRTEM, AFM) and spectroscopic (Raman, PL) techniques. We have calculated the electronic band structure and density of states of both samples. Fabricated devices were irradiated with different wavelengths (300-1100 nm) of light, showing outstanding responsivity with low dark current and a high on/off ratio. Timeresolved photocurrent measurements were also performed, which exhibit a fast response time. We also have designed photodetectors using multiscale modeling to explore the device's performance. By using semiconductor module for theoretically modeled devices, the terminal current across the device with respective wavelength was calculated and compared with the experimental results.

#### Mn-Doped CsPbBr<sub>3</sub> perovskites for Luminescent Solar Concentrators and Photocatalysis

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Lead Halide perovskites have been studied extensively for their diverse applications, especially in photovoltaics and photocatalysis. The excited charge carriers in Mn doped CsPbBr<sub>3</sub> have been reported to have longer decay lifetimes due to formation of manganese energy states in the bandgap of perovskite. The recombination of carriers through the Mn states produce low energy PL emission. In this work, we report the synthesis and embedding of Manganese doped CsPbBr<sub>3</sub> nanocrystals in PMMA polymer, as potential candidates for absorption free luminescent solar concentrators. Furthermore, we also investigate the charge carrier dynamics of Mndoped CsPbBr<sub>3</sub> nanocrystals (as sensitizers) coupled with Titanium di oxide (photocatalyst) nanostructures. Such systems are expected to have enhanced photocatalytic activity, owing to type-II band alignment, and availability of long-lived carriers for charge transfer and redox reaction. Mn-doped CsPbBr<sub>3</sub> nanocrystals were synthesized by hot injection method and characterized by UV-visible absorption, steady state and time resolved photoluminescence spectroscopy, X-ray diffraction and Transmission electron microscopy.

# Dielectric nanoantennas for optical studies on colloidal TMDC nanosheets

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The integration of plasmonic nanoantennas is a common way to improve optical and optoelectronic systems. As these antennas are made from noble metals, they suffer from ohmic losses, heating and are rather costly. Yet high index dielectric or semiconductor nanostructures are emerging as a promising alternative without these downsides [1]. They are likewise able to manipulate light at the nanoscale, and the resonant Mie-like modes, excited in the nanoantennas, support not only electric but also magnetic modes. Periodically arranged into a lattice (see Fig. 1a)), additional collective modes arise that are tunable by the excitation angle and lattice period. A field enhancement over a larger area and narrow linewidths can be achieved this way. Another advantage is, that these antennas can be made from well-studied materials, like silicon, wherefore the integration into semiconductor fabrication is feasible.

We aim to combine these arrays with two-dimensional materials, particularly transition metal dichalcogenides (TMDCs), like  $MoS_2$  and  $WS_2$ , to study their interaction like photoluminescence enhancement, redirected emission or strong coupling. Instead of the rather well known TMDC systems from exfoliation or vapor growth methods, we utilize wet-chemically synthesized colloidal TMDC nanosheets [2]. Scalable quantities of solution-based processable TMDCs, that show photoluminescence (see Fig. 1b)), can be obtained with this synthesis approach.



**Figure 1:** a) Image of a silicon nanoantenna array. b) Photoluminescence spectrum of WS<sub>2</sub> nanosheets.

- [1] I. Staude et al., ACS Photonics 6(4) 802-814 (2019)
- [2] A. P. Frauendorf et al., The Journal of Physical Chemistry C **125**(34) 18841-18848 (2021)

#### Exciton Dynamics in Perovskite Nanocrystal Superlattices with Different Interparticle Distance

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Perovskite nanocrystals synthesized with narrow size distributions are the perfect building blocks to assemble highly ordered meso-materials called superlattices. In recent years, collective phenomena such as superfluorescence have been reported in these materials.[1] Since then, many efforts have been spent trying to understand and control those effects, and fundamental research is still needed.

These collective phenomena arise from excitonic coupling across nanocrystals located in close proximity (e.g., dipole-dipole or dipole-electromagnetic field). Therefore, interactions are strongly dependent on the mutual distance between particles, meaning that the achieving a control over the inter-nanocrystal spacing might allow to control the collective response of the superlattices, collective effects, as suggested in theoretical works.[2] This is now possible thanks to recent advances in synthesis and surface chemistry of CsPbBr<sub>3</sub> nanocrystals, which allow to engineer their surface by introducing different ligands.[3] In this work, we will compare the impact of two surface capping agents of different length (i.e., oleylamine and octylamine) on the photoluminescence dynamics of nanocrystals in solution and after they have been assembled into superlattices.

Motivated by the need of understanding the energy flow and interactions between excitons across nanocrystals, we performed temperature- and fluence-dependent streak camera measurements (e.g. Figure 1), which highlighted a dependency of the photoluminescence temporal decay on the emission wavelength. We tentatively explain such trends based on the mobility of exciton across nanocrystals when in solution (i.e., isolated) and when self-assembled into superlattices, that is when tuning the ligands length has impact of the coupling efficiency.



**Figure 1**: Measured spectrally resolved dynamics of the photoluminescence of perovskite superlattices including a sketch of the hypothesized photophysics.

- [1] Rainò G., et al. (2018). Superfluorescence from lead halide perovskite quantum dot superlattices. Nature 563.7733 (671-675
- [2] Nguyen T. P., Tan L. Z., & Baranov D. (2023). Tuning perovskite nanocrystal superlattices for superradiance in the presence of disorder. J. Chem. Phys., 159(20)
- [3] Filippi U., et al. (2024). Cooling-induced order-disorder phase transition in CsPbBr<sub>3</sub> nanocrystal superlattices. ChemRxiv preprint. https://doi.org/10.26434/chemrxiv-2024-5q319

#### Direct Observation of Hole Drift and Diffusion in Contacted Nanowires Under Local Illumination

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Kelvin probe force microscopy (KPFM) is a method for measuring the surface potential. Being based on atomic force microscopy, KPFM enables investigating nanostructures, such as nanowires and nanosheets. Combining optical, electrical, and KPFM measurements in one setup enables advanced investigations of the charge-carrier separation in these materials and the properties of semiconductor-metal interfaces.

We investigate individual electrically contacted CdS nanowires, by combining scanning photocurrent mapping (SPCM) and KPFM. The charge-carrier mobility information of SPCM extended by KPFM maps gives a more complete picture of the path and hurdles, the charge carriers take inside the nanodevice in operando.

We show that upon local optical excitation, differences in charge-carrier mobilities of electrons and holes lead to an imbalance in the surface potential. At the point of illumination, positive charges accumulate, due to their lower mobility. KPFM reveals this imbalance and how it influences the potential drop along the biased CdS nanowire. Furthermore, performing KPFM while optically exciting the probed sample position monitors the excess of positive charge carriers for each position of the illuminated nanowire. A decrease of this excess shows how holes drift and diffuse into the contacts, where they contribute to the measured photocurrent.