PROGRAM

Bad Honnef Physics School 2023

Exciting nanostructures: Characterizing advanced confined systems

30 July - 4 August 2023, Physikzentrum Bad Honnef

Organized by Christian Klinke (University of Rostock) and Nikolai Gaponik (TU Dresden)

Sunday, 30 July 2023

17:00 – 21:00	*Registration*
18:30	DINNER / Informal get together

Monday, 31 July 2023

08:00	BREAKFAST
08:45 – 09:00	*Opening and welcome* Prof. Christian Klinke
09:00 – 10:15	*Colloidal Nanocrystals and Light* Prof. Jochen Feldmann (LMU Munich)
10:15 – 10:45	COFFEE BREAK
10:45 – 12:00	*Shape Control in Colloidal Synthesis Using Organic Ligands* Prof. Iwan Moreels (Ghent University)
12:00	**Conference Photo (in front of the Physikzentrum)**
12:15	LUNCH
14:30 – 15:45	*Theory and Computation of Semiconductor Nanostructures* Prof. Steven Erwin (Naval Research Laboratory)
15:45 – 16:15	COFFEE BREAK
16:15 – 17:30	*Flash talks by the students* Each talk has 2 min with 1 slide on their subject/poster
18:30	DINNER

Tuesday, 1 August 2023

08:00	BREAKFAST
09:00 – 10:15	*Synthesis and Optoelectronic properties of 2D Nanocrystals* Prof. Iwan Moreels (Ghent University)
10:15 – 10:45	COFFEE BREAK
10:45 – 12:00	*X-ray diffraction with spatial resolution* Dr. Ivan Zaluzhnyy (University of Tübingen)
12:15	LUNCH
14:30 – 15:45	*The Surface Science of Nanocrystals and MXenes* Prof. Dmitri Talapin (University of Chicago)
15:45 – 16:15	COFFEE BREAK
16:15 – 17:30	*Transport Properties of Thermoelectric Materials:* *Exploring the Pathways for Efficient Energy Conversion* Dr. Maria Ibanez (IST Austria)
18:30	DINNER
19:30	**Poster session 1**

Wednesday, 2 August 2023

08:00	BREAKFAST
09:00 – 10:15	*Beyond Conventional Quantum Dots* Prof. Celso de Mello Donega (Utrecht University)
10:15 – 10:45	COFFEE BREAK
10:45 – 12:00	*Highly Luminescent Lead Halide Perovskite Nanocrystals* Prof. Maksym Kovalenko (ETH Zurich)
12:15	LUNCH
14:00 – 18:00	Excursion & Café (hike in the vicinity, boat trip in case of rain)
18:30	DINNER (at the Physikzentrum)
19:30 – 21:00	**Meet the Editor(s)** Prof. Maksym Kovalenko (ETH Zurich and Associate Editor of *ACS Chemistry of Materials*) Prof. Dmitri Talapin (University of Chicago and Associate Editor of *RSC Chemical Science*)

Thursday, 3 August 2023

08:00	BREAKFAST
09:00 – 10:15	*Spectroscopic characterization of luminescent nanomaterials* Dr. Christian Würth (BAM, Berlin)
10:15 – 10:45	COFFEE BREAK
10:45 – 12:00	*Testing without Touching: Time-Resolved Terahertz-Spectroscopy for Nanostructures* Prof. Jannika Lauth (University of Tübingen)
12:15	LUNCH
14:30 – 15:45	*Magnetooptics of Nanostructures* Dr. Elena Shornikova (University of Dortmund)
15:45 – 16:15	COFFEE BREAK
16:15 – 17:30	*Nanostructures in electronic applications* Prof. Vanni Lughi (University of Trieste)
18:30	DINNER
19:30	**Poster session 2**

Friday, 4 August 2023

08:00	BREAKFAST
09:00 – 10:15	*Semiconductor Nanocrystal Optoelectronics using Colloidal Quantum Wells for Lighting and Displays: Pushing the Limits, Breaking Records* Prof. Hilmi Volkan Demir (Bilkent University)
10:15 – 10:45	COFFEE BREAK
10:45 – 12:00	*Nanomaterials for light harvesting* Dr. Ryan Crisp (University of Erlangen)
12:00 – 12:15	*Poster awards and closing remarks* Prof. Christian Klinke
12:30	LUNCH

End of the physics school and Departure

Nanomaterials for light harvesting

Ryan Crisp

Chemistry of Thin Film Materials,
Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Controlling the physical dimensions of a material in the nanometer size range enables certain emergent properties to be adjusted and optimized for the goal of converting the energy of light into other forms. The properties that prove the most interesting are related to not just quantum confinement effects but the surface-to-volume ratio as well as the electronic and structural nature of the nanomaterials' surface and overall geometry. We will cover in this lecture topics spanning nanostructuring for all manner (photo)electrochemical devices that will link the various materials properties discussed in the preceding talks of the workshop to their application. We will start with geometrical considerations of anodized aluminum oxide (AAO) membranes and nanospheres for structural color and move to control of the exposed atomic lattice planes for controlling the surface environment and finally end with more advanced light-matter interactions like multiple exciton generation – all relating to device applications.

Semiconductor Nanocrystal Optoelectronics
using Colloidal Quantum Wells for Lighting and Displays:
Pushing the Limits, Breaking Records

Hilmi Volkan Demir

NTU Singapore – Nanyang Technological University, School of Electrical and Electronic Engineering, School of Physical and Mathematical Sciences, Schoolof Materials Science and Engineering, Singapore

Bilkent University UNAM, Department of Electrical and Electronics Engineering, Department of Physics, Institute of Materials Science and Nanotechnology,Ankara, Turkey

Lighting and displays are integral parts of human activities and economic development. Semiconductor nanocrystals, now offering a market volume exceeding 1 Billion Euros annually, have attracted great interest in quality lighting and displays in the last decade. Such colloidal semiconductors enable enriched color conversion essential to superior lighting and displays. These colloids span different types and heterostructures of semiconductors, starting in the form of colloidal quantum dots about three decades ago and extending to the latest sub-family of nanocrystals, the colloidal quantum wells, in the last decade. In this talk, we will present most recent examples of photonic structures and device architectures using the colloidal quantum wells [1-5] for lighting and displays. Also, we will present a powerful, large-area, orientation-controlled self-assembly technique for orienting these colloidal quantum wells either all face down or all edge up [6]. We will demonstrate three-dimensional constructs of their oriented self-assemblies with monolayer precision [7]. Among their extraordinary features important to applications in lighting and displays, we will show record high efficiency from their colloidal LEDs [8] and record gain coefficients from their colloidal laser media [9] using heterostructures [2-5] and/or oriented assemblies [6,7] of colloidal quantum wells. Given their current accelerating progress, these solution-processed quantum wells hold great promise to challenge their epitaxial thin-film counterparts in semiconductor optoelectronics in the near future.

References

[1] B. Guzelturk *et al.,* HVD, Nano Letters **19**, 277 (2019)
[2] Y. Altıntas *et al.,* HVD, ACS Nano **13**, 10662 (2019)
[3] N. Taghipour *et al.,* HVD, Nature Communications **11**, 3305 (2020)
[4] F. Shabani *et al.,* HVD, Small **18**, 2106115 (2022)
[5] E. G. Durmusoglu *et al.,* HVD, ACS Nano in press (2023)
[6] O. Erdem *et al.,* HVD, Nano Letters **19**, 4297 (2019)
[7] O. Erdem *et al.,* HVD, Nano Letters **20**, 6459 (2020)
[8] B. Liu *et al.,* HVD, Advanced Materials **32**, 1905824 (2020)
[9] J. Maskoun *et al.,* HVD, Advanced Materials **33**, 2007131 (2021)

Beyond Conventional Quantum Dots

Celso de Mello Donegá

Debye Institute for Nanomaterials Science,
Utrecht University, Princetonplein 1, 3584 CC Utrecht, The Netherlands

Colloidal semiconductor nanocrystals are versatile nanostructures, whose properties are determined by their size, shape, composition, and compositional profile (*i.e.*, single component, gradient or homogeneous alloy, doped, heterostructured). In recent years, the synthesis of colloidal nanocrystals has reached a very mature level, owing to several decades of extensive research. The ability to control the size, shape and composition of these nanomaterials has grown dramatically, yielding a plethora of 0-dimensional quantum dots, 1-dimensional nanorods and nanowires, and 2-dimensional nanostructures, as well as more complex and sophisticated morphologies, such as multipods, nanorings, concentric core/multishell quantum dots, core/shell and Janus-type heteronanorods, and heterodimers. Their surface chemistry can also be tailored, allowing one to take full advantage of nanoscale effects to combine size-, shape- and composition-dependent properties with easy surface manipulation and solution processing. However, most of these developments have been restricted to Cd- and Pb-chalcogenide based nanocrystals. Unfortunately, the use of these nanostructures is severely limited by the intrinsic toxicity of Cd and Pb. This has motivated a worldwide research effort on alternative materials based on non- (or less) toxic elements.

In this lecture, I will focus on two promising alternative classes of materials: compound copper-chalcogenides (*e.g.*, I-III-VI_2 semiconductors such as $CuInS_2$) and III-V semiconductors (*e.g.*, InP, InAs, InSb). Several strategies have been used in the quest for high-quality colloidal nanocrystals and hetero-nanocrystals of these compounds, but their synthesis has proven to be far more challenging than that of their conventional counterparts. To allow these challenges to be properly appreciated and understood, I will first address the fundamental physical-chemical principles needed to understand the formation of colloidal nanocrystals and heteronanocrystals from a classical perspective. Subsequently, I will move beyond classical concepts to discuss the relevance of non-classical phenomena (*e.g.*, extended nucleation, non-classical nucleation, magic-size nanostructures, aggregative growth, cation exchange) to the preparation of unconventional quantum dots and (hetero)nanocrystals.

Theory and Computation of Semiconductor Nanostructures Steve Erwin, Center for Computational

Steven Erwin

Materials Science, Naval Research Laboratory, Washington DC

This lecture will provide an overview of the theory of semiconductor nanostructures. The "theory of nanostructures" encompasses theoretical ideas and methods from three different fields—physics, chemistry, and materials science. Numerical results usually require a fourth tool: computer calculations such as density-functional theory or quantum chemistry. Because most research is very specialized, many scientists have expertise in at most one or two of these four areas. The lecture will start with the basics and illustrate concepts using examples from current research, to help everyone gain a better understanding of all four aspects of the theory of nanostructures. Distribution Statement A. Approved for public release, distribution is unlimited.

Colloidal Nanocrystals and Light

Jochen Feldmann

Nano-Institute Munich, Physics Department, LMU Munich

In this lecture important results of colloidal nanocrystal (NC) research will be presented with a focus on their optical properties. Energy landscapes for electrons and excitons, the dynamics of optically generated excitations and changes induced by external fields will be addressed. In particular, the ever-growing number of semiconductor materials for the synthesis of NCs has considerably enriched the toolbox to tune many structural, electronic and phononic properties. Equally important, core-shell heterostructures, chemical and biochemical functionalization as well as hybrid nanosystems have led to a broad spectrum of novel effects and to important application scenarios.

Transport Properties of Thermoelectric Materials: Exploring the Pathways for Efficient Energy Conversion

Maria Ibáñez

Institute of Science and Technology (IST) of Austria, Am Campus 1, 3400 Klosterneuburg, Austria

Thermoelectricity is the phenomenon of converting heat directly into electricity and vice versa, offering a sustainable path to produce electricity from waste heat. As energy harvesters, thermoelectric devices can be used to partially recover large quantities of the waste heat (approximately 60% in developed countries) to reduce our primary energy production or to run low-power devices, especially those that require autonomy, such as sensors and transmitters in remote or difficult-to-access locations. Furthermore, its reversible nature allows thermoelectric devices to be operated as precise coolers for small-scale temperature control. Such localized cooling is crucial in infrared detectors, microelectronics, and optoelectronics, among others, where space is limited, and heat dissipation is localized.

This lecture will provide a comprehensive introduction to thermoelectricity. We will begin by giving a brief history of thermoelectrics, a description of the phenomenon, and its potential applications. Later on, we will introduce the fundamental principles of thermoelectricity, emphasizing the importance of material properties, in particular, those related to electronic and thermal transport. We will present the thermoelectric figure of merit and its significance as a metric for evaluating thermoelectric efficiency. ZT components, including electrical conductivity, Seebeck coefficient, and thermal conductivity, and their interplay in determining the overall performance will be deeply evaluated, and the different strategies to maximize performance will be presented using, as examples, traditional thermoelectric materials.

We will see that achieving high-performance thermoelectric materials requires synthesizing complex materials where not only the crystal structure but also other structural features such as defects, grain size, and orientation, and interfaces must be controlled. Hence, we will discuss the different strategies explored to produce thermoelectric materials and dive deep into the new opportunities that can be brought into the field by employing colloidal nanocrystals.

In summary, this lecture will offer a general view into thermoelectricity, shedding light on the principles, materials, advancements, and applications of this fascinating field, with an emphasis on the current research trends and future directions on the use of colloidal nanocrystals.

Highly Luminescent Lead Halide Perovskite Nanocrystals

Maksym V. Kovalenko

ETH Zürich, Department of Chemistry and Applied Biosciences, CH-8093, Zurich, Switzerland

Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600, Dübendorf, Switzerland

We will discuss the most recent addition to the family of colloidal semiconductor nanocrystals – those made of lead halide perovskites (LHP NCs) of composition APbX3 (A=Cs+, FA+, FA=formamidinium; X=Cl, Br, I). LHP NCs exhibit spectrally narrow fluorescence, tunable over the entire visible spectral region of 400-800 nm and high photoluminescence quantum efficiencies. Owing to their high oscillator strength, slow dephasing (long coherence times of up to 80 ps), minimal inhomogeneous broadening of emission lines, and a bright triplet exciton character with orthogonal dipole orientation, these NCs make for a highly versatile platform for creating controlled, aggregated states exhibiting collective phenomena. Their surface chemistry vastly differs from more conventional nanocrystals in that the capping ligands bind in non-covalent manner. Along with the structurally soft NC cores, non-covalent capping poses sever challenges. We will discuss various strategies for surface-functionalization, focusing on zwitterionic capping ligands represented by a broad family of synthetic phospholipids.

Testing without Touching:
Time-Resolved Terahertz-Spectroscopy for Nanostructures

Jannika Lauth

Institute of Physical and Theoretical Chemistry, University of Tübingen,
72076 Tübingen, Germany

Pump-probe (time-resolved) spectroscopic methods are excellent techniques for characterizing and understanding the photophysics and charge carrier dynamics of nanostructures. In this lecture, I will present an introduction to time-resolved terahertz spectroscopy (TRTS) and its use as all-optical method for non-contact photoconductivity measurements as well as for gaining information about bound excitons and free charges in nanostructures.

Shape Control in Colloidal Synthesis Using Organic Ligands

Iwan Moreels

Ghent University/Belgium

Shape control in colloidal nanocrystals took a disruptive leap forward in the year 2000, with the synthesis of anisotropic CdSe nanocrystals. Since then, it has been demonstrated in numerous materials, and we are now able to synthesize 1D nanorods, nanowires, even tetrapods, and octapods, or 2D nanodisks and extended nanosheets. In this lecture, I will discuss how we can gain control over these shapes by virtue of the organic ligands and their unique surface chemistry. More specifically, they can exhibit facet-dependent binding strengths that can be used to trigger anisotropic growth rates. On the other hand, through formation of micelles or lamellar structures, they can also serve as soft organic templates that direct crystal growth in specific directions.

Synthesis and Optoelectronic properties of 2D Nanocrystals

Iwan Moreels

Ghent University/Belgium

Next to shape control using organic ligands, 2D nanocrystal growth can also be obtained through facet-dependent energy barriers for nucleation and growth of additional layers on top of a nanocrystal. I will discuss this anisotropic growth mechanism introduced in 2017 for 2D CdSe nanocrystals and merge it with concepts introduced in the first lecture, to show how you can still exploit ligand surface chemistry to influence the 2D nanocrystal thickness, and lateral aspect ratio. Some of their unique opto-electronic properties, such as the giant oscillator strength and the large exciton binding energy, will also be introduced.

Magnetooptics of Nanostructures

Elena Shornikova

Experimental Physics 2, TU Dortmund University, Dortmund, Germany

Optical studies of colloidal nanocrystals at cryogenic temperatures (typically 1.7–4 K) and in high magnetic fields (typically above 10 T) provide valuable information about their emission properties. Exciton fine structure and lifetime, trion charge, g-factors and other parameters can be obtained from these measurements.

This lecture will give an overview of magnetooptical phenomena, which can be used to address spins of charge carriers and excitons in colloidal nanocrystals. I will show how exciton fine structure can be visualized by time-resolved polarized photoluminescence and fluorescence line narrowing. Second, I shall discuss pump-probe techniques, like transient absorption and Faraday rotation, as well as Raman spin-flip and optically detected magnetic resonance, and how they can be used to study the properties of nanostructures. In the end of my talk, I will make a short overview of magnetic properties of nanocrystals, which arise from doping with magnetic impurities and surface magnetism.

The Surface Science of Nanocrystals and MXenes

Dmitri V. Talapin

Department of Chemistry, James Franck Institute, and Pritzker School of Molecular Engineering, University of Chicago, Chicago, Illinois 60637, United States

This lecture will discuss modern approaches to structural design, description, and properties of surfaces in zero- and two-dimensional functional nanomaterials, specifically nanocrystals and MXenes, with some emphasis on their applications for electronics and optoelectronics.

The surface science of colloidal nanocrystals

The development of synthetic methods for well-defined colloidal nanostructures has introduced new routes for engineering functional materials via synthesis and assembly of nanoscale building blocks. All nanomaterials share a common feature of large surface-to-volume ratio, making their surfaces the dominant player in many physical and chemical processes. Surface ligands, molecules that bind to the surface, are an essential component of size and shape control during the nanocrystal synthesis, processing, and application. Understanding structure and properties of nanoscale surfaces requires an intricate mix of concepts and techniques borrowed from surface science and coordination chemistry. I will elaborate these connections and discuss the bonding, electronic structure, and chemical transformations at nanomaterial surfaces.

Colloidal nanocrystals offer an appealing manufacturing strategy that combines advantages of crystalline inorganic semiconductors with inexpensive solution-based device fabrication. Semiconductor nanocrystals are explored as the functional elements in commercial TVs and displays, printable electronics, light emitting devices, photodetectors and solar cells. By using optimized surface chemistries, nanocrystal arrays can exhibit high carrier mobilities and other characteristics appealing for electronic, thermoelectric and photovoltaic devices. The development of photochemically active surface ligands for colloidal nanocrystals enabled advanced additive manufacturing methods, such as direct optical lithography of functional inorganic nanomaterials.

The surface science of MXenes

Two-dimensional (2D) transition-metal carbides and nitrides (MXenes) show impressive performance in applications, such as supercapacitors, batteries, electromagnetic interference shielding, or electrocatalysis. These materials combine the electronic and mechanical properties of 2D inorganic crystals with chemically modifiable surfaces, and MXenes represent an ideal platform for fundamental and applied studies of interfaces in 2D functional materials.

I will discuss general strategies to install and remove MXene surface groups by performing substitution and elimination reactions. Successful synthesis of MXenes with oxo-, imido-, thio-, seleno-, or telluro-terminations, as well as bare MXenes (no surface termination), and hybrid organic-inorganic MXenes are demonstrated. MXene surface groups control biaxial lattice strain, phonon frequencies, electrochemical performance, the strength of electron-phonon coupling, making MXene surfaces not spectators but active contributors to conductivity, superconductivity and catalytic activity.

Spectroscopic characterization of luminescent nanomaterials

Christian Würth

Federal Institute for Material Research and Testing (BAM), Division Biophotonics, D-12489 Berlin, Germany

The rational synthesis of functional nanomaterials and nanomaterial optimization rely on the accurate characterization of many application-relevant features, ranging from particle size, size distribution and morphology over surface chemistry to more application-relevant features. This includes optical, electrochemical, and/or magnetic properties. In the following, spectroscopic methods for the measurement of the key spectroscopic performance parameters of nanomaterials like semiconductor quantum dots, luminophore-stained polymer and silica nanoparticles, and lanthanide-based nanocrystals with UV/vis/NIR/SWIR emission are presented. This includes the relative and absolute measurement of the photoluminescence quantum yield of these linear and non-linear emitters and the determination of particle brightness. In this context, also the calibration of fluorescence instruments and examples for common sources of uncertainty of photoluminescence quantum yield measurements are presented.

X-ray diffraction with spatial resolution

Ivan A. Zaluzhnyy

University of Tübingen

Thanks to their short wavelength, X-rays can resolve the structure of matter at the atomic level. This property has been extensively used to study crystal lattices since the beginning of the 20th century, and the vast majority of crystal structures have been characterized by X-ray diffraction. Nowadays, thanks to the development of bright synchrotron sources, we can use intense nanofocused X-ray beams with tunable energy. This makes X-rays a very important tool for characterizing the structure of novel nanoscale materials and devices.

At the beginning of the lecture, we will discuss the basics of X-ray diffraction and crystallography. In the second part, we will discuss recent advances of X-ray synchrotron sources and the possibility of using a nanofocused X-ray beam to study the structure of nano-objects with spatial resolution. As examples, we will consider X-ray scattering from self-assembled mesocrystals and resistive-switching nanodevices.