Science is not about believing; science is about logic, knowledge and questioning.

Third International Perovskite Workshop in Lund: "Multi-Timescale Dynamic Processes in Metal Halide Perovskites: From Fundamentals to Applications"

September 23 – 24, 2024, Lecture Hall G, Chemical Center, Sölvegatan 39, Lund

Organizers

Ivan Scheblykin (Chemical Physics, Lund University), ivan.scheblykin@chemphys.lu.se

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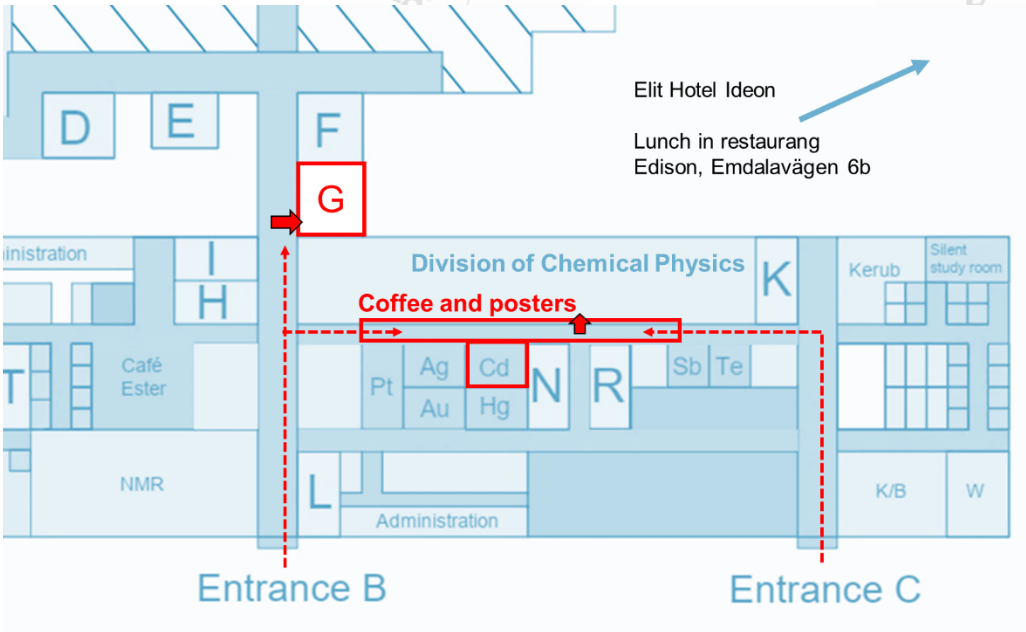
Sponsors:

- The Swedish Research Council (Vetenskapsrådet)
- Lund University, NanoLund
- Lund University, Chemistry Department, Division of Chemical Physics

Each invited talk has 50 min slot of which about 25 minutes are reserved for discussion.
Posters will be presented during the long coffee breaks on day 2.

Location:



More info to navigate:
https://www.chemphys.lu.se/news/perovskite-workshop-2024/

Program

Day 1. Sep 23, 10.00 – 17.30

1. **David Cahen** (Weizmann Institute of Science, Israel)
Photovoltaic Materials and Structural (Dis)Order

Questions for discussion:

- Is decades too short a timescale for a field to grow up?
- How does dynamic disorder affect static disorder, our beloved, elusive (illusive?) structural imperfections?
- What are critical timescales for material resilience / ability to handle damage?
- HaPs as a part of an evolution of disorder in (PV) materials
- Damage-resistance of HaPs combining features at different time scales
- The Achilles heel and front door for electronic property control of HaPs.

2. **Ivan Scheblykin** (Chemical Physics, Lund University)
The Concept of a Dynamic Semiconductor and its State.

Defect types and their concentrations in metal halide perovskites are not the characteristics given the sample preparation. Indeed, preparation is very important, however it is by far not the end of the story. This is a crucial difference to most of other semiconductors. Depending on the external stimuli like light irradiation, voltage, current *etc*. these characteristics changes and evolve in time. Because defects are the key players determining the semiconductor properties, their dynamics influence results of all optical and electrical measurements. So, when we do a series of experiments (e.g. change light intensity, current, etc) we essentially probe different states of the material because the material adjusts to the experimental conditions.

Questions for discussion:

- What is the magnitude of this problem? Do the experiments published over 10 years make sense at all?
- When the defects are not stable and constantly appear and disappear, can it be the main reason of so-called defect tolerance known for perovskites?
- Is there is any way to stabilize the materials in one state or another during optical experiments?
- Can these defect dynamics be used for any applications?

Coffee break

3. **Hannes Hempel** (Helmholtz-Zentrum, Germany)
Time-Resolved Energy Losses and Photoluminescence in Lead Halide Perovskite

Questions for discussion:

- How do processes beyond carrier recombination cause trPL decays and how can they be identified?
- What is the charge carrier lifetime under constant solar illumination?
- Is non-radiative recombination of higher-order dominating?
- How large are the defect concentrations in halide perovskites?
- What can we learn from the trPL amplitude?
- Does trPL measure the time-resolved Fermi level splitting?
- How do geminate carriers influence photoluminescence and do they contain extra free energy?

Lunch

4. Thomas Kirchartz (FZ Juelich, Institute for Energy and Climate Research, Germany).
Extracting Diffusion Lengths from Transient Photoluminescence Measurements

Questions for discussion:

- How relevant is the diffusion length as a figure of merit for charge collection?
- What causes power law decays and how universal are they?

5. Juan F. Galisteo Lopez (Instituto de Ciencia de Materiales de Sevilla, Spain).
Understanding Carrier Recombination in QD Solids: Doubts and Certainties

Time resolved spectroscopies are routinely employed to study carrier recombination in lead halide perovskites providing valuable insight into different processes from carrier cooling to charge trapping/detrapping and radiative recombination. Most studies are usually carried out on morphologies amenable to be simulated with existing theoretical models such as single crystals, thin films or nanocrystals. Over the past few years we have focused on the study of carrier recombination in a system of interest for optoelectronic applications: quantum dot (QD) solids. In particular we have explored their photophysical properties as inter-QD separation is varied. This allows us to tune the electronic coupling among QDs and thus we can transition from an ensemble of independent QDs to an array of interconnected QDs showing signatures of free-carrier transport.

As conventional models (Shockley-Read-Hall, ABC model) fail to reproduce time-resolved measurements in these systems, we propose an alternative way of representing these data that allows to extract valuable information from the character of recombination (mono- or bi-molecular) to recombination rates (band to band recombination). Further, we have explored the role of the surrounding atmosphere as a means to provide information on the nature of defects present in halide perovskites (both, QD solids and thin films) and also on the influence of defects on carrier recombination in the above systems.

Questions for discussion:

- Signatures of quantum confinement and free carrier recombination are present in QD solids: how can we bring both pictures together?
- How much information can the surrounding atmosphere (in the absence and presence of external irradiation) provide on the nature of defects in halide perovskites?
- Can we obtain a valuable insight (regarding carrier trapping, diffusion, etc.) from deviations of TRPL data from Shockley-Read-Hall predictions?

Coffee break

6. Ziming Chen (*Department of Chemistry, Imperial College London, UK*).
Possible Non-Radiative Recombination Processes in Perovskite Solar Cells

Questions for discussion:

Should we consider the effect of electron-phonon coupling in non-radiative recombination?

- What does the activation energy obtained from the Arrhenius fit of temperature-dependent PL intensity signify?
- In trap-assisted recombination, how can we assess the trap filling and recombination process?
- Do we need to rely solely on modelling, or are there experimental approaches to investigate these processes?

Lab tours
Dinner

Day 2. Sep 24, 10.00 – 17.30

7. Juan Bisquert (UPV, Valencia, Spain)

Hysteresis in Perovskites and Applications of Memory Effects

Hysteresis, observed in the current-voltage characteristics of electronic and ionic devices, is a phenomenon in which the shape of the curve is influenced by the speed of measurement. This phenomenon is a result of internal processes that introduce a time delay in the response to external stimuli, causing measurements to depend on past disturbances. Hysteresis and time delay effects find important applications in devices that are explored for resistive switching and neuromorphic computation, such as halide perovskite and organic memristors and transistors for synapses and neurons.
Here we discuss the memory effect in halide perovskite solar cells and memristors, emphasizing functional models that can describe complementary dynamical measurements like time transients and impedance spectroscopy. We show the application of these approaches to determine rapidly the performance of high-quality perovskite solar cells. we explain the operation of perovskite memristors as synapses in computational networks.

Questions for discussion:

- What is the chemical-material basis of the observed delay effects (beyond ion-induced effects, more concrete mechanisms)?
- Can we apply the interaction of light and current to the memory mechanisms, light-driven?

Coffee break and Posters

8. Simon Kahmann (University of Cambridge, UK; TU Chemnitz, Germany)

Broad Emission Bands in Halide Perovskite-Inspired Materials – Current Understanding and Open Questions

Questions for discussion:

- What are the roles of self-trapped excitons, native defects, and dopants?
- How do we distinguish between proposed mechanisms?
- Do broadbands always result from localized transitions and what is the time required for localization?
- Why are some transitions narrow and others broad?
- What are the involved phonons?
- Why can broad emission bands be bright if they result from defects?
- What regulates their lifetimes?
- What is the difference between a Frenkel exciton and a self-trapped exciton?

Lunch

9. Tönu Pullerits (Chemical Physics, Lund University)

Different Timescales in Perovskites – from Hot Carrier Cooling to Trap States and Their Dynamics

Photoinduced dynamics in perovskites and their nanostructures occur at a very broad range of timescales – from fast subpicosecond hot carrier cooling to milliseconds and slower processes related to trap states and their dynamics. Many of these processes are discussed as being relevant for the perovskite applications as photovoltaic and light emitting materials. For example, the prospects of using the material for hot carrier solar cells has been extensively discussed in literature. We will present our recent work on the topic touching the outstanding questions below.

Questions for discussion:

- How slow should be the hot carrier cooling for making the hot carrier solar cell viable
- prospect?
- Should we think electronic cooling or vibrational cooling in the context of hot carrier solar cells?
- How to characterize the trap states and their dynamics?
- Does temperature dependence of PL give additional useful information
- There are many different trap states – are the "effective" models which include only one, maybe two, useful?

10. Silvia Motti (University of Southampton, UK).
THz Spectroscopy in The Investigation of Perovskite Lattice Softness

I will discuss the role of lattice dynamics in the optoelectronic properties of perovskite semiconductors, and how optical spectroscopy can be applied to investigate it. We have used THz spectroscopy to detect photoinduced phonon shifts that evidence the link of anharmonicity with phase segregation in mixed halide perovskites, and we have demonstrated the rapid drop in conductivity during the formation of excitons and polarons observed by simultaneous THz and transient absorption measurements. The experimental evidence provides critical insights, but quantitative analysis and precise modelling are beyond reach. Open questions remain regarding phonon anharmonicity and its role in perovskite photophysics.

Questions for discussion:

- How do we disentangle intrinsic effects from extrinsic factors such as defects and grain boundaries?
- How can we explore the compositional space of perovskites to control lattice softness and mitigate its detrimental effects?

Coffee break and Posters

11. Prashant V. Kamat (University of Notre Dame, USA).

How Ion Migration in Metal Halide Perovskites Impacts Solar Cell Performance

The ability to tune the bandgap of metal halide perovskites through compositional alloying of the halide ion is of interest in designing tandem solar cells and light emitting displays. However, photoinduced migration of halide ions can significantly affect the device performance. One such property is photoinduced phase segregation in mixed halide perovskites (MHP), which forms bromide rich and iodide-rich domains. These domains act as charge carrier traps and lower the efficiency of perovskite-based devices. The thermodynamic and redox properties of halide perovskites provide a strong driving force for hole trapping and oxidation of iodide species. These iodide species interact with hole transport layer, such as SpiroOMeTAD, changing its oxidation state. Thus, the mobility of halides and their susceptibility to hole-induced oxidation play a crucial role in determining the long-term stability of metal halide perovskite solar cells. The need to suppress halide ion migration as well as cation migration to achieve long term stability and improve efficiency of perovskite solar cells will be discussed.

Questions for discussion:

What is the meaning of "Highly efficient and Stable"? Why do we continue to use this phrase to define PSC, when we are aware of its instability. (We have been using this phrase for more than 10 years)

- There have been several surface treatment strategies reported in the literature to achieve performance stability of PSC?
- Is there a single strategy that we all can employ?
- How can we standardize PSC stability testing protocols so that results from different stability can be compared?

Closing remarks
Lab tours
Self-organized dinner

Poster presentations

1. Performance Fluctuations in Tin Perovskite Solar Cells

Miriam Minguez-Avellan[1], *Omar E. Solis*[1], *Pablo F. Betancur*[1], *Pablo P. Boix*[2]

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[2] Instituto de Tecnología Química, Universitat Politècnica València-Consejo Superior de Investigaciones Científicas, Av. dels Tarongers, 46022, València, Spain.

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2. Perovskite metal halide single crystals as a promising platform for long endurance and high performance memristor devices

Ismael Fernandez-Guillen [1], *Clara A. Aranda* [1,2], *Pablo F. Betancur* [1], *Marta Vallés-Pelarda* [1], *Cristina Momblona* [1,3,4], *Teresa S. Ripolles* [1], *Rafael Abargues* [1], *and Pablo P. Boix* [1]

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[3] Instituto de Nanociencia y Materiales de Aragón (INMA) CSIC-Universidad de Zaragoza Department of Chemical and Environmental Engineering Campus Río Ebro-Edificio I+D Universidad de Zaragoza C/ Mariano Esquillor S/N, Zaragoza 50018, Spain
[4] Centro de Investigación Biomédica en Red de Bioingeniería, Biomateriales y Nanomedicina Instituto de Salud Carlos III Zaragoza 50018, Spain

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3. Dye-Modified Interfaces in Perovskite Solar Cells used as Probe

Svea M. Stepping and Gerrit Boschloo

Department of Chemistry, Ångström Laboratory, Uppsala University, Uppsala, SE-75120 Sweden

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4. Identifying Recombination Resistance and its Impact on Current-Voltage Curve Reconstruction in Perovskite Solar Cells

Pablo F. Betancur[1], *Omar E. Solis*[1], *Rafael Abargues*[1], *Teresa S. Ripolles*[1], *and Pablo P. Boix*[2]

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5. Excitation Dynamics in Perovskite Solar Cells Probed by Photocurrent Detected 2D Spectroscopy

Edoardo Amarotti [1], *Luca Bolzonello*[2], *Sun-Ho Lee*[3], *Donatas Zigmantas*[1], *Nam-Gyu Park*[3], *Tõnu Pullerits*[1]

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[2] ICFO—Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Castelldefels, Barcelona 08860, Spain
[3] School of Chemical Engineering, Sungkyunkwan University, Suwon 16419, Korea

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6. Impact of Atomic Layer Deposition Tin Oxide Properties on the Characteristics of Perovskite Solar Cells

Bhavya Rakheja[1], *Fredrik Larsson*[2], *Adam Hultqvist*[1], *Tobias Törndahl*[1], *Erik Wallin*[2]

[1] Uppsala University, Uppsala, Sweden.
[2] First Solar ETC, Uppsala, Sweden.

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7. Controlled Ligand-Free Growth of Free-Standing CsPbBr3 Perovskite Nanowires

Ziyun Huang[1], *Zhaojun Zhang*[1], *Nils Lamers*[1], *Dmitry Baranov*[2], *Jesper Wallentin*[1]

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[2] Division of Chemical Physics and NanoLund, Department of Chemistry, Lund University, Box 124, Lund, 22100, Sweden.

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8. Engineering Luminescent Metal Halide Nanomaterials at the Nanochemistry and Spectroscopy Group in Lund

Dmitry Baranov, *Yong Li*, *Lorenzo Tallarini*, *Matheus G. Ferreira*, *Chenxu Jiao*, *Stefano Toso*

Division of Chemical Physics and NanoLund, Department of Chemistry, Lund University, P.O. Box 124, Lund, SE-221 00, Sweden

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9. Memlumor – A Luminescent Memory Device for Energy-Efficient Photonic Neuromorphic Computing

Alexandr Marunchenko[1], *Jitendra Kumar*[1], *Alexander Kiligaridis*[1], *Dmitry Tatarinov*[2], *Anatoly Pushkarev*[2], *Yana Vaynzof*[3,4], *Ivan G. Scheblykin*[1]

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[4] Leibniz-Institute for Solid State and Materials Research Dresden, Helmholtzstraße 20, 01069

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10. Hidden Photoexcitations Probed by Multi-Pulse Photoluminescence

Alexandr Marunchenko[1], *Jitendra Kumar*[1], *Dmitry Tatarinov*[2], *Anatoly Pushkarev*[2], *Yana Vaynzof*[3,4], *Ivan Scheblykin*[1]

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11. Ultrafast Charge Trapping at Buried Interface in Perovskite Solar Cells Revealed by Optical-Control with Surface Photovoltage Detection

Beier Hu[1], *Tiankai Zhang*[2], *Haoqing Ning*[1], *Tong Wang*[1], *Jiaxin Pan*[1], *Feng Gao*[2], *Igal Levine*[3], *Ziming Chen*[1], *Artem Bakulin*[1,*]

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[2] Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, SE-58183, Sweden
[3] Institute of Chemistry and The Center for Nanoscience and Nanotechnology, Hebrew University, Jerusalem, 91904, Israel

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12. Impact of Charge Carrier Diffusion and Trapping on the Photoluminescence Decays in Metal Halide Perovskites

Jitendra Kumar[1], *Alexandr Marunchenko*[1], *Alexander Kiligaridis*[1], *Shraddha M. Rao*[1], *Ankur Yadav*[2], *Oscar Telschow*[3], *Monojit Bag*[2], *Thomas Kirchartz*[4], *Yana Vaynzof*[3], *Ivan G. Scheblykin*[1]

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[3] IEK-5 Photovoltaik, Forschungszentrum Jülich, Jülich, Germany
[4] Technical University of Dresden, Dresden, 01069, Germany

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13. Unveiling Mechanism of Temperature-Dependent Self-Trapped Exciton Emission in One-Dimensional Hybrid Organic-Inorganic Tin Halide for Advanced Thermography

Yanmei He [1], *Xinyi Cai* [2], *Xiaochen Wang* [3], *Mikkel Baldtzer Liisberg* [4], *Jakub Dostál* [5], *Muyi Zhang* [2], *Miroslav Kloz* [5], *Feng Gao* [2], *Tönu Pullerits* [1], *Junsheng Chen* [4]

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[5] *ELI Beamlines Facility, The Extreme Light Infrastructure ERIC, Za Radnicí 835, 25241 Dolní Břežany, Czech Republic*

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14. How to probe light induced defects in MAPI thin films? The usage of long pulses in time resolved photoluminescence

Maxim Simmonds [1], *Thomas Dittrich* [2], *Thomas Kirchartz* [3], *Rowan MacQueen* [1], *Eva Unger* [1]

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[2] Young Investigator Group Nanoscale Solid-Liquid Interfaces, Chemical Energy Division, Helmholtz Zentrum Berlin
[3] IEK-5 Photovoltaik, Forschungszentrum Jülich, Jülich, Germany

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15. Phase Segregation and Ion Migration in $MAPb(I_{0.4}Br_{0.6})_x$ Perovskite Films with Varying Stoichiometries ($2.94 \leq x \leq 3.06$)

Fulya Koc [1], Nathaniel P. Gallop [1], Juanzi Shi [1], Fabian Paulus [1], Yana Vaynzof [1,2]

[1] Leibniz-Institute for Solid State and Materials Research Dresden, 01069 Dresden, Germany
[2] Chair for Emerging Electronic Technologies, TUD Dresden University of Technology, 01187 Dresden, Germany

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16. First-principles calculations shed light onto the electronic structure and dynamics of organic-inorganic perovskite analogues

Kostas Fykouras [1] *and Linn Leppert* [1]

[1] MESA+ Institute for NanotechnologyUniversity of Twente, Netherlands

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17. Optical and Vibrational Properties in Quantum Confined 2D Lead Halide Perovskites Nanocrystals

Mustafa Aboulsaad [1], *Rafael Araujo* [1], *and Tomas Edvinsson* [1]

[1] Ångström laboratory, Uppsala University, Sweden

18. Coherent Phonons and Charge Carrier Localization in Cesium Gold Bromide

Sankaran Ramesh[1], *Yonghong Wang*[2], *Pavel Chabera*[1], *Rafael Araujo*[3], *Mustafa Aboulsaad*[3], *Tomas Edvinsson*[3], *Feng Gao*[2], *Tönu Pullerits*[1]

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