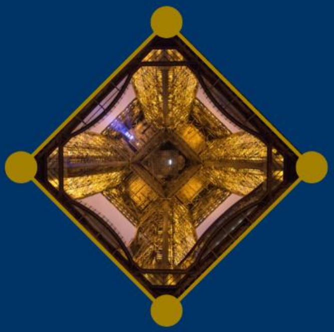
JPH 2026

Ile-de-France, 4 - 6 May 2026

Journées Pérovskites Halogénées 2026



Saint-Lambert, 4 - 6 May 2026

Book of abstracts

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JPH 2026
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Poster 18	PRISM: Benchmarking Halide Perovskite Single Crystals for X- and Gamma-Ray Spectrometric Imaging – Teresa Stefanini – CEA LETI
Poster 19	Random Lasing in All-Inorganic Perovskite $CsPbBr_3$ Metasurface – Vui Nguyen – INL
Poster 20	Scalable pulsed laser deposition of $CsPbI_3$ for perovskite-on-silicon tandem solar cells – Elvire Guillerm-Cottenceau – CEA LITEN
Poster 21	Semiempirical DFTB Approaches for 3D and 2D Perovskites and Their Heterostructures – Sreejith Pallikkara Chandrasekharan – Institut FOTON
Poster 22	Study of $CsPbBr_3$ color conversion layers fabricated by PLD for color conversion in microLED displays – Natalia Zambrano Ortega – CEA LETI
Poster 23	Unveiling Clusteroluminescence in a Two-Dimensional Organic-Inorganic Hybrid Perovskite for Tunable Optical Properties – Kawthar Abid – Université de Lorraine

Halide perovskites : synthetic aspects and powder X-ray diffraction characterization

Nicolas Mercier*[1]

[1]Nicolas MERCIER – MOLTECH-Anjou, University of Angers – France

Résumé

This tutorial focuses on the synthetic aspects of halide perovskite (HP) materials and their characterization using powder X-ray diffraction (PXRD). The preparation of HP in the form of crystals, crystallized powders, or thin films will be covered.
First, the different types of perovskites will be reviewed: 3D, 2D, or 3D-2D systems (thin films).

Regarding synthesis techniques from solutions, the characteristics/properties of common solvents (dielectric constant, (a)polar and (a)protic character, Gutmann factor, etc.) will be described first, before the various crystallization methods (cooling, evaporation, liquid-gas diffusion, solvothermal, etc.) are described. The preparation of thin films by spin-coating, particularly 2D-3D systems, will be covered. Solvent-free synthesis techniques will also be discussed, including solid-state synthesis (ball milling, heating) and molten-state synthesis (when congruent melting occurs).
The principles of X-ray diffraction by matter will be reviewed, followed by an examination of the experimental aspects of powder X-ray diffraction (PXRD). Finally, examples of PXRD of HP samples and their analysis will be reviewed, including thin film systems.

Mots-Clés: halide perovskites, synthesis, X, ray diffraction

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*Intervenant

Defect properties in halide perovskites

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Résumé

We will present the different kind of electronic defects and their impact on semiconductor properties. The characteristics of defects in hybrid perovskites are key to such a boom with perovskite solar cells and other optoelectronic devices. We will present different electrical and optical techniques that are important to identify and quantify the defects. We will highlight the defect tolerance with respect to charge transport properties. Another limitation in perovskites related to low defect-formation energy is ion migration, which will also be addressed in this tutorial lecture.

Mots-Clés: defects, optical, electrical, ion migration

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*Intervenant

Defects Activity in Metal Halide Perovskites

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[1]Istituto Italiano di Tecnologia (IIT) – Via Morego, 30 16163 Genova, Italie

Résumé

Metal halide perovskites make an appealing material platform for a new generation optoelectronic technology. One superior feature is their tunable bandgap by designing the chemical composition of the crystalline unit. In this lecture I will assess the most recent advances in elucidating the (photo)chemistry of defects related to the chemical composition of the perovskite crystalline unit. I will show how they define the charge carrier dynamics in the semiconductor. Based on such understanding I will discuss the main electrical and spectroscopic features related to the activity of defects and how to exploit them to improve the figures of merit of optoelectronic devices and their stability.

Mots-Clés: perovskites, semiconductors, defects

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[*] Intervenant

Advanced Functionalities of Perovskite Nanocrystals Embedded in Nanoporous Scaffolds

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[1]Instituto de Ciencia de Materiales de Sevilla – Espagne

Résumé

Synthesizing perovskite quantum dots (PQDs) within nanoporous matrices offers a promising alternative to traditional colloidal methods. These matrices feature a controllable network of voids, acting as nanoreactors in which precursor solutions can be infiltrated. Further thermal or chemical treatments convert them into nanocrystals. This confinement enables precise control over PQD dimensions, size distribution, and crystallinity without requiring stabilizing ligands. This talk highlights the method's potential to enhance PQD stability and functionality and to study fundamental properties of both individual QDs and QD networks. Key advantages include: (i) Stabilization of metastable phases, like the α-phase of CsPbI3 even at room temperature; (ii) Control over the environmental responsiveness; (iii) High optical performance, with quantum yields exceeding 85% for specific compositions such as FAPbBr; (iv) Versatility for low-dimensional Structures, as the approach extends to fabricating low-dimensional perovskite structures, enabling remarkable blue photoluminescence with quantum yields surpassing 40% or the formation of exciton-polaritons; (v) Efficient charge transport within the embedded QD network, which depends critically on achieving PQD interconnectivity to enable dot-to-dot charge transfer, key for successful device operation.

Mots-Clés: Perovskite nanocrystals, perovskite quantum dots, advanced functionalities, photonics

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*Intervenant

Quantum light from colloidal lead-halide perovskite quantum dots

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[2]Swiss Federal Laboratories for Materials Science and Technology [Dübendorf] – Switzerland

Abstract

Understanding and controlling light emission lies at the heart of a broad range of classical and quantum light applications. An emerging, technologically scalable material platform for this end is colloidal metal-halide perovskite quantum dots (QDs).
In this talk, I will discuss the exciting photophysics of perovskite QDs from a quantum-light perspective, presenting several examples based on single-particle spectroscopy and *ab-initio* molecular-dynamics simulations from the Kovalenko lab. On the one hand, perovskite QDs feature even larger crystal softness and more pronounced electron-phonon coupling than their bulk parent compound. On the other hand, these soft QDs host superior quantum-light emission, including high single-photon purity, near-blinking-free emission(1), and high color purity(2). A further peculiarity is their strikingly dissimilar photophysics at cryogenic and room temperature. At cryogenic temperature, perovskite QDs behave as textbook semiconductors, capable of cavity-free coherent quantum-light emission and even hosting phenomena such as single-photon superradiance(3) and superabsorption(4). At room temperature, on the other hand, coupling of the exciton to large-amplitude lattice vibrations in the QD core and at the QD surface induces dynamic partial exciton wavefunction localization(5), a process limiting the coherence but increasing the single-photon purity(6).

References:

(1) V. Morad, et al., *Nature* **2024**, 626, 542-548.

(2) G. Rainò, et al., *Nat. Commun.* **2022**, 13, 2587.

(3) C. Zhu, et al., *Nature* **2024**, 626, 535–541.

(4) S.C. Boehme, et al., *Nat. Photonics* **2025**, 19, 864–870.

(5) L.G. Feld, et al., *Nat. Commun.* **2026**, 17, 1974.
(6) C. Zhu, et al., *Nano Lett.* **2022**, 22, 3751–3760.

Keywords: quantum light, perovskite, quantum dot, nanocrystal, exciton, phonon coupling, single, particle spectroscopy

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Invited 3

Upscaling perovskite growth using hybrid or full vacuum methods for perovskite/silicon tandem solar cells

Solenn Berson*[1,2], Kilian Alcocer[2], Kristell Carreric[2], Helen Bristow[2], Polyxeni Tsoulka[2], Elvire Guillerm-Cottenceau[2], Louis Grenet[2], and Florian Dupont[2]

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Résumé

In the last ten years, tandem solar cells based on perovskite (PK) materials have shown promising results, surpassing the theoretical limits of single junction Silicon (Si) solar cells. Even though PK/Si tandem solar cells appear capable of achieving $> 35\%$ of power conversion efficiency, many challenges need to be overcome in order to upscale the PV devices from 1 cm^2 laboratory scale to larger areas. With that perspective, vapor deposition of the absorber layer seems promising in order to elaborate a conformal and high quality perovskite on top of textured industrial silicon wafers. In the literature, the main industrially compatible techniques to grow the PK layer can be divided into two axes: i) PK deposition by full vapor deposition techniques and ii) PK deposition by hybrid processes.
In a first part, we propose pulsed laser deposition (PLD) as full vacuum scalable method to fabricate uniform black phase inorganic perovskites. We first developed several PLD-grown contact layers (ITO, SnO2 and NiOx), and then demonstrated the deposition of CsPbI2Br and CsPbI3 on 300 mm wafers, exhibiting PL peaks at λ=648 nm (_˜1.91 eV) and 700 nm (_˜1.77 eV) respectively. Final device integration and performance measurements are currently underway.

In a second part, we focus on a hybrid deposition process combining thermal co-evaporation, close space sublimation (CSS) and solvent step for the elaboration of organic-inorganic perovskite layer. Using different characterization techniques, we investigate the structural and chemical properties of the inorganic scaffold. The goal of this study is to understand how the homogeneity, the porosity and the composition of the first layer affect the growth of the final PK film. Simultaneously, we examine the key factors that influence the crystallization mechanism during the second wet step.
Final part will be dedicated to the stability assessment of tandem architecture under outdoor and accelerated ageing conditions.

Mots-Clés: perovskite/silicon tandem solar cells, scale up process

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*Intervenant

Reproducibility of perovskite optoelectronic devices at the laboratory scale

Johann Bouclé*[1]

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Résumé

For over a decade, halide perovskites have emerged as a game-changer in photovoltaic energy conversion, achieving power conversion efficiencies that rival those of monocrystalline silicon. Advances in exploring various dimensionalities and compositions have also extended their impact to other fields, including light emission, detectors, fuel cells, etc. However, despite these high-performance achievements, major challenges persist-primarily in stabilizing device performance and improving the reproducibility of large-scale processes.
In this context, I will briefly illustrate how ambient conditions can rapidly compromise the reproducibility of quasi-2D perovskite light-emitting diode (LED) fabrication processes in gloveboxes at the laboratory scale. Specifically, I will highlight how minor temperature fluctuations and atmospheric contamination can lead to significant dispersion in phase composition.

Additionally, while chlorine-based additive engineering is a critical strategy for achieving high-efficiency perovskite solar cells, the extreme process sensitivity and associated reproducibility challenges-observed in some cases-are rarely addressed in the literature. To further illustrate these constraints, I will analyze the impact of the widely used methylammonium chloride (MACl) additive on perovskite solar cell performance. In particular, I will discuss observations of bimodal photoluminescence behavior in perovskite active layers processed with MACl. I will demonstrate that the resulting irreproducibility in device performance can be attributed to compositional and structural heterogeneities, including halide-rich phase coexistence and non-uniform micro-strain distributions. Transitioning from MACl to alternative additives that mitigate these non-uniformities appears to be a robust strategy for enhancing device reliability at the laboratory scale.

Q.-H. Do, R. Antony, B. Ratier, J. Bouclé, "Improving Device-to-Device Reproducibility of Light-Emitting Diodes Based on Layered Halide Perovskites", Electronics 13(6) (2024) 1039*
V. Viswakarman, M. Garcia Rocha, J. Bouclé, "Methylammonium Lead Chloride as a Robust Additive for Reproducible Perovskite Solar Cells", submitted manuscript*

Mots-Clés: reproducibility, perovskite optoelectronic devices, solar cells, light, emitting diodes, structural inhomogeneities

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*Intervenant

Automating PV Research from Experimentation to Data Analysis.

Vincent Le Corre*[1]

[1]University of Southern Denmark – Danemark

Résumé

Photovoltaics (PV) research is experiencing a paradigm shift driven by advances in automation, artificial intelligence, and machine learning (ML). The field is shifting from manual, labor-intensive exploration of chemical space to self-driving laboratories.
In this presentation, I will discuss both the opportunities and the challenges associated with these emerging workflows. I will demonstrate how robotic platforms guided by ML algorithms can enable the development of high-performance perovskite solar cells within days rather than months.

I will also introduce the open-source software package **optimPV**, a flexible framework designed to address key challenges in solar cell research, including intelligent experimental planning and the fitting of high-dimensional physical models to experimental data. By minimizing user intervention, this approach accelerates device optimization and enables robust extraction of critical physical parameters in perovskite and organic semiconductor devices. The capabilities of this methodology will be illustrated through several case studies employing different physical models and experimental techniques, including (i) transient photoluminescence and microwave conductivity, (ii) light-intensity-dependent current–voltage measurements, and (iii) voltage-dependent absolute photoluminescence.

Mots-Clés: Perovskite Solar Cells, Machine Learning, Modeling, Self driving laboratories

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*Intervenant

Bismuth-based halide perovskites confined in mesoporous matrices for CO2 photoreduction

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Résumé

Lead-free halide perovskites have several advantages over lead-based ones such as much lower toxicity and higher ambient stability. However, they are usually much less stable under the conditions of photocatalytic CO2 reduction. Moreover, their charge generation is usually somewhat inefficient due to the lack of catalytically active sites. In this work, space-confined nanocrystals of stable Cs3Bi2X9 (X = Br, I) were synthesized in the pores of SiO2 mesoporous matrices (1) and tested in solid/gas photocatalytic CO2 conversion. We will discuss the properties of the confined perovskites and their influence on the photocatalytic performance.

A combined experimental/theoretical study highlights an unprecedented CH4 production yield achieved. Coupled with a very high selectivity of $> 80\%$, it makes these materials one of the best among all halide perovskite photocatalysts for CH4 production. We will discuss and compare the performance of different confined bismuth halide perovskites, bulk perovskite powders, as well as the size of the pores and the effect of the confinement. We will show that the unique combination of the increased density of active surface sites and high concentration of reactant molecules around nanocrystals in the pores are at the origin of the high performance and selectivity.

Other types of confined perovskites and other photocatalyses, such as organic tranformations, will be equally discussed.

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*Intervenant

(1) Dupé, S.; Liu, D.; Ghosh, A.; Vasenko, A. S.; Pouget, S.; Schlutig, S.; Vidal, M.; Lebeau, B.; Ling, W. L.; Reiss, P.; Prezhdo, O. V.; Ryzhikov, A.; Aldakov, D. Quantum-Confined Bismuth Iodide Perovskite Nanocrystals in Mesoporous Matrices. Nanoscale 2024, 16 (23), 11223–11231.

Mots-Clés: lead, free perovskites, photocatalysis, CO2 photoreduction, mesoporous matrices

Growth dynamics and properties of thin MaPbI3 layers prepared in UHV

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Résumé

Vacuum deposition of thin layers of organic-inorganic hybrid perovskites appears to be a valuable alternative to the solution-based method ((1)). Although this approach allows for better control of the growth process, it presents a number of difficulties. The transition to ultra-high vacuum, which is necessary to obtain higher purity layers, paradoxically introduces an additional complication due to the very significant reduction in the partial pressure of water ((2)).

Using an original approach combining several techniques operating in real time during growth (structural characterization by fast atom diffraction, optical characterization by differential reflectivity spectroscopy, partial pressure monitoring by quadrupole mass spectrometry), we have access to the growth dynamics of thin MAPbI3 layers on a silver and graphene substrates. The effective production of MAPbI3 layers is only possible by significantly increasing the MAI/PbI2 flux ratio to a value of 600, compared to a typical ratio of 4 under vacuum conditions dominated by water vapor. On graphene, although the layer does not show crystalline character, it is perfectly identified by its absorption bands and gap. Good quality single-crystal layers with a tetragonal structure are observed on the silver substrate. We also observe the inevitable initial formation of 2 to 3 pure PbI2 monolayers before the appearance of the MAPbI3 phase. Low-temperature micro-photoluminescence measurements show a main peak at 1.61 eV and a weaker peak at 1.65 eV, in relative agreement with the results in the literature.

(1) Mingzhen Liu et al.; Nature 501, 395 (2013). https://doi.org/10.1038/nature12509

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*Intervenant

(2) A. Allouche et al., J. Phys. Chem. C 2025, 129, 18737–18748. https://doi.org/10.1021/acs.jpcc.5c04748

Mots-Clés: Vapor deposition, UHV, hybride perovskites, MAPbI3

Mechanosynthesis of hybrid perovskite composite as an electromagnetic wave absorber

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Résumé

The development of ever-increasing means of communication, such as 5G, and detection systems, such as military and civilian radars, is leading to an increase in the number of sources emitting electromagnetic waves and thus in strong electromagnetic pollution. This pollution can be the source of numerous interference problems between devices, as well as possible health problems. In that context, there is a strong need for new absorbent materials that are more effective and also over a wider frequency range. Hybrid perovskites (HPs) are excellent dielectric materials with many polarisation modes that can be modulated according to frequency, making them excellent candidates for electromagnetic wave absorption (EMWA) application. However, EMWA testing requires a large quantity of powder to be dispersed within a polymeric matrix. Therefore, hybrid perovskites were synthesised using mechanosynthesis, a solvent-free method that enables the production of large quantities of powders with good reproducibility and homogeneity. The most studied HP, MAPbI, showed promising EMWA properties but suffers from poor air stability. We therefore have studied the mechanosynthesis of other compositions, such as CsPbBr and MAPbBr, exhibiting a higher stability. They demonstrated new promising EMWA properties at the X band, 6 to 13 GHz and also Ku band, 13 to 20 GHz. However, these HPs need further combination with dielectric and magnetic materials to be considered EMWA materials. To adjust their absorbing properties, we have combined these HPs with carbon-based materials to introduce new dissipation mechanisms, particularly interfacial polarisation and charge dissipation networks. We chose to work with graphene due to its conductive properties and its ability to form good interfaces with HPs. Tests were carried out to determine the best way to integrate graphene into the synthesis process, the optimal ratio. We have characterised them structurally and optically (band gap, photoluminescence) to correlate these properties to their EMWA properties.

Mots-Clés: Hybrid Perovskite, Electromagnetic Wave Absorption, Mechanosynthesis

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Enhancing the stability of metal halide perovskite thin films during ALD-SnOx deposition using amino-silane interlayers.

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Résumé

Solar cells based on metal halide perovskite (MHP) represent an emerging and promising thin film technology within the field of photovoltaics, yet they are limited by their poor stability against extrinsic species. To act as a moisture barrier and shield the MHP from sputter-related damage, atomic layer deposited (ALD) coatings, notably SnOx, are added on top of the MHP. However, typical ALD processes induce a degradation of the photo-absorber, leading to cells with $< 1\%$ efficiency, which stresses the need for a protection of the MHP film during the ALD process We propose in this work the introduction of an ultra-thin protective organic layer through the evaporation of 3-(2-Aminoethylamino)propyltrimethoxysilane (AEAPTMS), which was successfully used as a passivation layer on double cation perovskite by Lin et al. (2024, Science), onto a triple cation perovskite (Cs0,05(MA0,16FA0,84)0,95Pb(I0,842Br0,158)3). First, we investigate the nature of the degradation taking place within the MHP when directly coated with ALD-SnOx, by exposing the MHP film to the ALD precursors, namely tetrakis (dimethylamido)tin(IV) (TDMASn) and to byproducts of the reaction. This highlighted the presence of new N-containing species through X-ray photoelectron spectroscopy, whose exact determination is still under investigation, and a near total quenching of the MHP photoluminescence. The impact of AEAPTMS exposure on the MHP film and its propensity to form a protective layer are then evaluated by proceeding to the SnOx deposition on the AEAPTMS coated MPH. With adequate optimization, AEAPTMS passivates

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the interface and leads to a protection of the MHP after TDMASn exposure, preventing PL quenching and leading to structural change within the MHP film, with the formation of a lower dimension perovskite denoted by XRD diffractograms. While full devices relying on AEAPTMS interlayers were characterized and did not show significant improvement, further investigation and optimization are required to assess the full potential of this interlayer.

Mots-Clés: Metal halide perovskite, Atomic layer deposition, Passivation, Interface chemistry, Photovoltaics

Talk 5

Optical spectroscopy of single CsPbBr perovskite quantum dots synthesized by a modified LARP method

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Résumé

Colloidal lead halide perovskite quantum dots (pQDs) have rapidly emerged as a versatile class of nanomaterials that combine the appealing optoelectronic properties of bulk perovskites with the advantages of quantum confinement (1). At the single dot level, pQDs exhibit stable single photon emission up to room temperature (2) and a 50% photon indistinguishability at cryogenic temperatures (3). This positions them among the very few colloidal emitters capable of combining high brightness, coherence, and quantum purity. However, to date, single pQD studies have relied almost exclusively on hot-injection synthesis (4), a process that demands stringent control of temperature and inert atmosphere, thus limiting scalability.

Here, we demonstrate that a modified ligand-assisted reprecipitation (LARP) method provides a robust and highly versatile alternative for producing single CsPbBr pQDs. Using a recently introduced amine-mediated trimming strategy (5), combined with didodecyldimethylammonium bromide (DDAB) ligands for enhanced surface passivation, we obtain isolated LARP-synthesized pQDs suitable for fundamental photophysical properties studies. High-resolution micro-photoluminescence experiments at cryogenic temperatures show a stable emission with minimal spectral diffusion of the bright exciton with its characteristic fine structure and its low-energy optical phonon replicas. Power-dependent studies also reveal the trion and biexciton states contributions. Time-resolved measurements demonstrate sub-100-ps radiative lifetimes, and photon-correlation experiments under CW and pulsed excitation confirm high-purity single-photon emission.

These results demonstrate that ligand-tailored LARP synthesis produces pQDs with intrinsic optical properties comparable to hot-injection counterparts, while offering great flexibility for post-synthetic ligand engineering. This versatility could be crucial for assembling pQDs into superstructures, in order to investigate collective quantum phenomena.

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Mots-Clés: Perovskite, Quantum Dots, Ligand Assisted Reprecipitation Synthesis, Single Particle Spectroscopy, Photoluminescence, Single Photon Source

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Buried perovskite quantum dots for quantum light electroluminescence

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Résumé

Halide perovskite quantum dots are a promising technological platform for quantum light emission. As colloidal nanocrystals, they have demonstrated near-unity photoluminescence quantum yield with weak blinking or spectral diffusion, short radiative lifetime close to their

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coherence time, and single-photon as well as entangled-photon-pair emission. In this talk, I will present a new class of perovskite quantum dots buried within a perovskite matrix displaying photoluminescence characteristics close to their colloidal counterpart, including clear spectral signatures of the exciton fine-structure and phonon sidebands. Single-photon emission is moreover demonstrated with electrical injection through the perovskite matrix. I will discuss how excitons and their fine-structure can be modeled by empirical effective-mass methods and how these calculations can help characterize the observed quantum dots.

Mots-Clés: quantum dots, quantum emission, theory, exciton fine structure

Investigation of hyperfine spin relaxation and dynamic nuclear polarization in lead halide perovskite polycrystalline films

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Résumé

For more than a decade, interest in metal-halide perovskites has grown due to their remarkable optoelectronic and photovoltaic properties, making them promising for solar cells and light emitting devices applications. Furthermore, lead-halide perovskites, like MAPbI3, exhibit a strong spin-orbit coupling and spin-selective optical transitions for potential spintronics applications. We investigated the relaxation of localized charge carrier spins in MAPbI3 polycrystalline films using time-resolved pump-probe Faraday Rotation (PFR) under a longitudinal applied magnetic field (Fig.1a). We show how these measurements can be used to characterise the hyperfine interaction in these materials, finally giving access to hyperfine correlation times and localization volumes (1). Furthermore, we showed that the hyperfine interaction induces a transfer of the charge carrier spin polarization to the nuclear spin system, creating a dynamic nuclear polarization (DNP). Spin polarization measurements as a function of the magnetic field reveal an asymmetric curve (Fig.1b), indicating that the nuclear spin polarization acts back on the charge carrier spins as an effective magnetic field adding up to the applied field (2)(3). Its magnitude increases with excitation density and we obtain a maximum Bn = 40mT for an excitation of 100mW/cm^2. We also show how the process of DNP itself can be asymmetric relative to the external magnetic field (3).
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Mots-Clés: Optical spin orientation, pump probe faraday rotation, hyperfine spin relaxation, dynamic nuclear polarization

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Talk 8

Spin noise of electrons and holes in Lead Halide Perovskite Crystals

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Résumé

Spin properties of charge carriers in lead halide perovskite crystals are of great interest for both fundamental research and practical applications. Typical experiments adressing spin properties involve measuring the magneto-optical response of the material to external perturbations. In this work, however, we adopt a different approach: spin noise (SN) spectroscopy, where spin properties are deduced from spontaneous fluctuations of magnetization. This technique has only recently been applied to perovskite nanocrystals. Here, we employ it to investigate thin films of MAPI single crystals, whose high structural quality has been confirmed by experiments demonstrating optical orientation of electron, hole, and nuclear spins.
Both electron and hole contributions are clearly identifiable in the SN spectra. Their spectral positions as a function of magnetic field allow us to confirm this identification based on the corresponding g-factors, while the spectral linewidths are related to the spin dephasing times. The latter appear to be as long as _˜10 ns at optimum conditions.

The temperature dependence of the spin dephasing times suggests that localization plays a more significant role in hole spin dephasing. Indeed, we observe an increase in the hole spin dephasing time from 6 nsat 3K to 9 ns at 7 K (a motional narrowing effect), whereas this behavior is not observed for electrons.
We analyze these results in terms of the interplay between hyperfine and spin-orbit interactions for electrons and holes in MAPI crystals.

Mots-Clés: spin, spin noise spectroscopy, MAPI

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Close Space Sublimation for perovskite-silicon tandem solar cells

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Résumé

Tandem perovskite-silicon solar cells have attracted tremendous attention due to their performances with certified efficiencies above 34%. These outstanding performances have been achieved using solution-based processes, which may be a hint towards industrialization, because of the inherent limitations of the liquid processes (solution waste management, scalability and conformal deposition on textured Si substrates).
To overcome these issues, vacuum based processes have been developed recently, such as co-evaporation or Close Space Sublimation (CSS). The CSS designation is however used in literature for very different processes with only the common feature of a short source-to-substrate distance. This designation actually covers:

- CSS deposition: a method to deposit material from a single source material (eg. CsPbBr3)

- CSS impregnation: a method to impregnate inorganic material with an organic compound (eg. using FAI to transform PbI2 to FAPbI3).

Both approaches are relevant for PV applications and can be used depending on the material to be synthesized. In this contribution we explore the potentiality of the CSS technique to fabricate perovskite-silicon tandem cells, using:

- CSS deposition of inorganic perovskite materials (CsPb(I,Br)3) have been explored as absorbers for tandem devices.

- CSS deposition of inorganic precursors (CsBr + PbI2) has been used as a first stage for the synthesis of hybrid CsFAPb(I,Br)3 photovoltaic absorbers

- CSS impregnation of inorganic precursors with FAI and FABr for the synthesis of hybrid CsFAPb(I,Br)3 photovoltaic absorbers
This contribution will focus on the potential, advantages and drawbacks of the CSS synthesis method (both deposition and impregnation strategies) for PV absorbers deposition with a particular attention paid on the physical mechanism underlying the CSS deposition process. Understanding the CSS deposition method is a prerequisite to determine the applicability of such a method and to be able to optimize device performances. This demonstration will be supported by solar cells fabrication and performances analysis.

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Mots-Clés: Close space Sublimation, CSS, tandem, solar cells

Terminal Group–Dependent Interactions in Carbazole-Based SAMs: Implications for Pb^2 Coordination and Interface Engineering in Perovskite Solar Cells

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Résumé

In recent years, interface engineering has emerged as a central strategy for overcoming non-radiative recombination and stability limitations in perovskite solar cells (PSCs), with self-assembled monolayers (SAMs) playing a key role as molecularly tunable interlayers between metal oxides and perovskite absorbers . In this context, this study investigates the influence of the terminal functional group of SAMs on interfacial properties and device performance in PSCs fabricated under ambient air conditions.
Two carbazole-based phosphonic acid SAMs, CHO-2PACz and NH-CH-2PACz, were employed as interfacial modifiers between the NiO hole transport layer (HTL) and the MAPI perovskite absorber. Such carbazole-based SAMs are widely recognized for their ability to tune work function, enhance hole extraction, and promote controlled perovskite growth, making them a benchmark in high-efficiency inverted PSC architectures.

The formation and organization of the SAMs were first confirmed by infrared spectroscopy and X-ray photoelectron spectroscopy, evidencing successful grafting and well-ordered molecular assemblies on the oxide surface. Ultraviolet photoelectron spectroscopy further revealed that the two SAMs induce distinct modifications of the interfacial electronic structure and NiO work function, highlighting the critical role of terminal group chemistry in energy level alignment.

Consistent with recent advances in SAM-mediated crystallization control, morphological and

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structural analyses show that SAM functionalization significantly improves perovskite film quality, leading to larger grains and reduced pinhole density. This effect is particularly pronounced for the amino-terminated SAM. A detailed investigation of the SAM/perovskite interface reveals that specific interactions between terminal groups (NH vs CHO) and Pb^{2} ions govern nucleation, defect passivation, and interfacial energetics, in agreement with previous reports on Lewis base–Pb^{2} coordination and surface defect mitigation.

Mots-Clés: Perovskite solar cells, Inverted architecture (p–i–n), Carbazole, based SAMs, MeO, 2PACz, NH, CH, 2PACz, hole transport layer, Interface engineering, Power conversion efficiency, stability

Contrôle de l'alignement énergétique aux interfaces des films de pérovskites halogénées 2D/3D et des couches de transport de charge

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Résumé

Malgré les progrès rapides des performances des cellules solaires à pérovskites, la stabilité des dispositifs demeure le principal obstacle à leur commercialisation. Celle-ci est fortement influencée par l'architecture du dispositif, la composition de la pérovskite et les interfaces avec les couches de transport de charge (CTL, charge transport layer). Récemment, la passivation de surface à l'aide d'hétérostructures de pérovskites bidimensionnelles/tridimensionnelles (2D/3D) a montré un potentiel considérable. Cependant, bien qu'un alignement de bandes favorable à ces interfaces soit souvent supposé améliorer la dynamique des porteurs de charge, sa vérification expérimentale directe reste limitée.

Dans ce travail, nous étudions l'énergétique d'interface de couches de pérovskites 2D formées avec des cations espaceurs d'iodure de 4-fluorophényléthylammonium (4-FPEAI) sur une pérovskite 3D à triple cation, en utilisant la spectroscopie de photoémission ultraviolette (UPS), la spectroscopie de photoémission des rayons X (XPS) et la spectroscopie de photoémission inverse (IPES). Nous examinons d'abord l'énergétique et les décalages de bandes en fonction de l'épaisseur de la couche 2D. Ensuite, une interface modèle pérovskite/CTL est étudiée par évaporation de couches de spiro-TTB d'épaisseur comprise entre 5 et 120 Å sur la structure 2D/3D.

Des calculs complémentaires de théorie de la fonctionnelle de la densité montrent que l'alignement des niveaux d'énergie dépend fortement de la terminaison de surface. Si des monocouches 2D ultraminces présentent un alignement favorable, des couches 2D plus épaisses peuvent induire des décalages de bandes qui entravent l'extraction des charges, en particulier pour les surfaces terminées au brome. Ces résultats ouvrent la voie à une conception rationnelle d'interfaces 2D/3D aux propriétés électroniques optimisées, améliorant à la fois l'efficacité et la stabilité.

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Mots-Clés: Pérovskites 2D/3D, Interfaces, Alignement de bande, Spectroscopie photoélectronique

Reduced Quasi-Fermi Level Splitting Deficit by Homogenizing Interfacial Photo-potential for Highly Efficient Perovskite Solar Cells

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Abstract

Quasi-Fermi level splitting (QFLS) deficit is widely recognized as the limiting factor of inferior open-circuit voltage (VOC) in perovskite solar cells (PSCs). However, a comprehensive understanding of its underlying mechanisms and effective mitigation strategies remain elusive. In this work, we systematically investigate the QFLS-VOC mismatch in inverted PSCs passivated with different single molecules between perovskite and electron transport layer, revealing a clear dependence on molecular structure (piperazine $>$ benzene $\approx$ thiophene) in both half- and full-stacking architectures. By correlating QFLS analysis with spatially resolved surface photovoltage (SPV) characterization, we demonstrate that the differentiated QFLS loss originates from the non-uniform SPV distribution induced by distinct passivation molecules. Meanwhile, we discover that a synergistic passivation strategy combining conjugated and non-conjugated compounds could effectively homogenize and enhance the SPV across the entire perovskite film. This uniform electrostatic landscape simultaneously suppresses the QFLS deficit and promotes efficient charge extraction. As a result, bi-molecules passivation through the combined use of piperazine- and a thiophene- derived iodides enables a champion power conversion efficiency (PCE) of 27.18% (certified steady-state PCE of 26.47%), together with outstanding operational stability. Notably, encapsulated large-scale (50.35 cm2) flexible devices, specifically optimized for stability, retained over 98% of their initial efficiency after 2450 h of continuous illumination.

Keywords: Quasi Fermi Level Splitting (QFLS), QFLS and Voc mismatch, surface photo voltage (SPV), binary molecules surface passivation, inverted perovskite solar cell (PSCs)

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*Speaker

Ferroelectric hybrid perovskites based semiconductors for optoelectronics

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Résumé

Hybrid Organic-Inorganic Perovskites (HOIPs) are a class of semiconductors consisting of an inorganic structural framework of lead-halide octahedra within which organic cations are embedded. Incorporating larger organic cations the octahedral connectivity can be tuned from 3D to 2D, 1D or 0D. In this work we address 2D HOIPs that display ferroelectricity, namely materials that possess a spontaneous polarization that can be reversed in the presence of a sufficiently large electric field. Ferroelectricity is a property deeply related to structural symmetry and the phase transition phenomena. Due to the great structural tunability they provide an excellent platform to investigate the origin and characteristics of ferroelectricity in HOIPs which could have applications on photovoltaics (1), spintronics (2) or photodetectors (3).

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Mots-Clés: Ferroelectricity, Lead Hybrid Perovskites, Structure, Property relations

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*Intervenant

Talk 14

Solution-Processed CsPbBr3-based Photodetectors: A Versatile and Robust Platform for Wearable Sensing

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Résumé

Metal halide perovskites have emerged as a compelling platform for optoelectronic sensing, combining the high performance of traditional semiconductors with the processing versatility of organic materials. In this work, we report a solution-processed CsPbBr3 photodetector specifically engineered for photoplethysmography (PPG) applications .
The device was fabricated through a low-temperature, printable process compatible with flexible substrates. Polymeric engineering of the perovskite solution was employed to optimise film morphology, leading to higher photocurrent and ensuring robustness against mechanical stress. Interfacial engineering with a PCBM electron transport layer further enhanced charge extraction and significantly suppressed noise, resulting in a responsivity of 1.9 A/W and an external quantum efficiency of 650% under green illumination. The photodetector exhibited fast temporal response (rise/fall times $\approx$ 500 μs), low dark current (_˜0.06 nA), and a specific detectivity of _˜3 $\times$ 10^{12} Jones at 1 kHz, demonstrating suitability for low-intensity physiological signal detection.

Integrated in a reflective-mode PPG configuration, the device was successfully employed for in-vivo heart-rate monitoring. Frequency-domain analysis enabled reliable heart rate extraction, with a 10-second acquisition window providing a practical compromise between spectral resolution (_˜6 bpm) and physiological heart rate variability . The recorded signals remained stable and repeatable in time and across different cardiac states of the subject.
These results demonstrate the feasibility of fully solution-processed CsPbBr photodetectors for wearable biosensing and highlight their potential for scalable, low-cost integration into flexible health-monitoring platforms.

Mots-Clés: Sensing, Photodetector, Flexible

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*Intervenant

Stabilization of the dark current in perovskite sintered X-ray detectors via 2D/3D surface functionalization

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Résumé

3D perovskites such as MAPbI3 have demonstrated remarkable performance for X-ray detection, achieving unprecedented sensitivity under X-ray and at low fabrication temperatures. However, they usually exhibit poor operational and environmental stability that severely limit their development to a commercial product. On the other hand, 2D perovskites such as PEA2PbI4 perform very well in terms of stability, but at the price of reduced charge transport properties. Here, we present an innovative fabrication approach that combines advantages of both 3D and 2D perovskites, while mitigating their drawbacks. A powder of a 3D methylammonium lead triiodide (MAPbI3) perovskite is soaked in a solution containing an appropriate amount of phenethylammonium iodide (PEAI) in isopropanol, resulting in surface-functionalized 2D/3D particles. The treated powder is then sintered to fabricate X-ray detectors that demonstrate enhanced sensitivity compared to the bare MAPbI3 material, as well as exceptional operational stability with reduced and stabilized dark current. This work introduces a novel approach to enhance the performance and stability of X-ray detectors made of lead halide perovskite materials.

Mots-Clés: 2D/3D perovkites, X, ray detectors, sintering, stabilization

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Semiconducting perovskites for medical X-ray radiography: environmental effects on chemical and electrical properties of CsPbBr3 detectors.

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Résumé

Since 2013, metal halide perovskites have been studied as a promising new material for X-ray detection in medical imaging. (1) Their use as thick layers ($> 100\ \mu$m) in direct X-ray detection devices could provide spatial resolution and sensitivity superiors to that of indirect scintillator-based detectors (1,2) and would allow for better medical diagnostic and reduced exposure dose for the patient. The fully inorganic CsPbBr3 is a candidate of choice due to its high atomic number providing good X-ray absorption. Moreover, CsPbBr3 shows improved chemical stability compared to organic halides perovskites (3). However, a deeper understanding of the physical and chemical properties of CsPbBr3 is still needed to improve device performance and reproducibility. In particular, unintentional extrinsic doping coming from impurities and from the working atmosphere. To this end, thick layers of polycrystalline films obtained by Physical Vapor Deposition (4) were exposed to different atmospheric conditions in order to understand their impact on the detector performances and pave the way for encapsulation studies.

Electrical properties such as dark and X-ray photo current were measured under both dry and humid atmosphere as well as in air and inert conditions. It was found that relative humidity is the main factor inducing changes in the material electrical properties. Furthermore, those changes in dark and X-ray photo current were found to be reversible with kinetics dependent on the humidity level. To obtain a deeper understanding of the chemical mechanism at play, photoluminescence and X-ray diffraction measurement under different humidity levels were carried out.

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Mots-Clés: Inorganic Perovskite, Xray detector, Humidity, Electrical measurments

Enhanced Photoluminescence of Cesium Lead Halide Perovskite Nanowires via Plasmonic Coupling

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Résumé

Photonic nanowires based on semiconductor materials have potential applications in the manipulation of light at the nanoscale and play a key role in the development of integrated photonic/electronic devices. To achieve the best optical performance for these applications, it is crucial to enhance the photon conversion efficiency of the nanowires. A promising way to enhance light emission from nanowires is to combine semiconductors with noble metals. The strong confinement of the electromagnetic field resulting from plasmonic structures can effectively transfer surface plasmon resonance energy to semiconductors via excited electrons and thus enhance the photoluminescence (PL) yield. Here, we report plasmon-enhanced light emission from a hybrid nanowire consisting of noble metal and semiconductor materials. The demonstration is performed in a cesium lead halide perovskite-based four-layer structure (CsPbBr3/PMMA/Ag/Si) designed to limit plasmonic losses in the metal while exhibiting efficient surface plasmon–photon coupling at moderate power. We employ temperature-dependent micro-photoluminescence spectroscopy (from 4 K to 300 K) to study the optical properties of the nanowires. The study, conducted with 100 fs laser pulses at a repetition rate of 76 MHz and at an excitation wavelength of 400 nm, reveals that a 5 nm thick PMMA layer and 7.5 nm sized Ag nanoparticles enhanced the PL intensity by approximately a factor of 29 compared to pure semiconductor structures at 4 K. In addition, we investigate the emission dynamics of carriers and excitons in the nanowires using time-resolved photoluminescence spectroscopy techniques. The observations show enhanced carrier recombination dynamics due to plasmonic interactions with the perovskite. These results show a potential way to excite hybrid nanowires at sufficiently low photon density so that single-photon excitation/emission could be possible from these structures.

Mots-Clés: Perovskites nanowires, plasmonics, helium droplets, micro photoluminescence spectroscopy

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Talk 18

Room-temperature Polariton Lasing in CsPbBr3 Perovskite Metasurfaces

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Abstract

Halide perovskites have recently emerged as an excellent platform for exploring exciton-photon strong coupling, leading to the formation of exciton-polaritons. Owing to their mixed light-matter nature, polaritons enable lasing at significantly lower thresholds than conventional photon lasers. Since the first demonstration in all-inorganic perovskite planar microcavities (1), progress has expanded to layered perovskites (2) and perovskite colloidal quantum dot microcavities (3). However, the conventional vertical microcavity architectures, which rely on thick distributed Bragg reflectors, provide limited flexibility for engineering emission directionality and spatial control of polariton modes.

Here, we demonstrate room-temperature polariton lasing using a CsPbBr polaritonic metasurface composed of CsPbBr single crystals with a patterned ZEP layer on top, which overcomes limitations by enabling precise control over the emission's directivity and polarization. The device exhibits highly directional lasing at normal emission (0○) with a low threshold of _˜0.3mJ.cm^{2} . The onset of polariton lasing is evidenced by the nonlinear increase of the emission, pronounced linewidth narrowing with a continuous blueshift (Fig.1d), and the buildup of long-range spatial coherence. These results represent a step toward low-threshold, highly controllable microscale polariton lasers.

Acknowledgments:

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Keywords: Polariton lasing, All, inorganic perovskite, CsPbBr3, Metasurface, Nanoimprint

Cartographie de la génération du photopotentiel et des pertes aux interfaces dans des cellules solaires pérovskites triple cation à halogénures mixtes sous conditions operando

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Résumé

L'amélioration des rendements des cellules solaires repose sur une compréhension approfondie et une maîtrise des processus fondamentaux incluant l'absorption des photons, la génération de paires électron–trou, la séparation, le transport et la collecte des porteurs de charge. Dans ce contexte, la qualité du matériau absorbeur et le contrôle des interfaces avec les couches de transport sont essentiels notamment via un bon alignement des bandes et une minimisation des recombinaisons non radiatives.
Dans ce travail, nous nous sommes intéressés à des cellules solaires à base de pérovskites halogénées, en particulier les alliages triple cation et halogénures mixtes (FA0.83MA0.12Cs0.05PbI2.55Br0.45), avec différentes couches organiques de passivation . L'objectif était d'étudier dans des conditions *operando* (sous illumination laser et sous polarisation électrique) leur stabilité chimique et optoélectronique.

Des mesures HAXPES (Photoémission à haute énergie) couplées à des mesures PL (photoluminescence) ont été réalisées sur la ligne de lumière GALAXIES du synchrotron SOLEIL.

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Une attention particulière a été portée en premier lieu à des mesures d'homogénéité et de stabilité du matériau absorbeur dans les conditions d'analyse en fonction de l'intensité des rayons X durs ($h = 6$ keV), de l'illumination laser (660 nm) et de la nature de la couche de passivation. Des polarisations directes et inverses ont ensuite été appliquées aux cellules, permettant la réalisation de mesures *operando* HAXPES/PL avec un enregistrement simultané des caractéristiques courant–tension.

Nous réalisons ces mesures HAXPES operando dans des géométries de dispositifs adaptées, avec des couches de transport ultrafines et des électrodes d'une épaisseur inférieure à 25 nm. Cette approche, combinée à des mesures couplées XPS-PL réalisées en laboratoire, nous permet de suivre les variations de la génération et des pertes de photopotentiel spécifiques aux éléments, et donc aux couches, et de les corréler à une diminution de l'intensité de photoluminescence qui correspond à un taux de recombinaison élevé.

Mots-Clés: Photoemission, HAXPES, Operando, Photoluminescence, Photopotentiel

Homogeneous All-Inorganic Perovskite Films via High-Pressure Recrystallization: Amplified Spontaneous Emission and Phase Transition Dynamics

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Résumé

Metal halide perovskite semiconductors have emerged as leading materials for optoelectronic devices, owing to their exceptional optical and electronic properties. Among them, all-inorganic perovskites such as CsPbBr3 have attracted substantial research due to their superior thermal and chemical stability compared to hybrid organic- inorganic counterparts (1-3). However, achieving high-quality CsPbBr3 thin films through solution-process without chemical engineering still remains a big challenge due the to the precursor's low solubility in common solvents. Recently high-pressure recrystallization has proven to be effective method to improve film quality, while its effect on film properties remains largely unexplored. In this work, we present a systematic investigation of the morphological, structural, and optical properties of CsPbBr thin films prepared via high-pressure recrystallization, in comparison with conventional non-recrystallized films (4). Optimized recrystallization at 300 bar yields smooth, pinhole-free, single-phase 3D perovskite layers with sub-nanometer roughness. Optical analyses reveal that the recrystallized films exhibit amplified spontaneous emission with a reduced excitation threshold and enhanced photostability. Furthermore, temperature-dependent X-ray diffraction uncovers the orthorhombic-tetragonal-cubic phase transitions in the recrystallized films, in good agreement with reports on single crystals in the literature. Overall, this study represents a promising step toward the development of cost-effective, large-scale devices for optoelectronic applications.

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Mots-Clés: All, Inorganic perovskites, recrystallization, homogeneous, crystallinity, amplified spontaneous emission

Tuning the structural and optoelectronic properties of metal halide perovskites by hydrostatic pressure

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Résumé

Pressure is a fundamental thermodynamic variable that governs the state and properties of materials. Changes in pressure can alter bond lengths and angles and may even induce transitions between different crystallographic phases. Hybrid metal halide perovskites are relatively soft, making their structures and properties especially sensitive to pressure variations. Structural distortions induced by pressure, such as octahedral tilting, bond compression, or symmetry changes, can significantly modify their electronic structure. In particular, pressure can tune the band structure and band alignment by altering orbital overlap and the relative positions of the conduction and valence bands. Moreover, pressure-induced structural asymmetry can influence spin–orbit coupling related phenomena, such as the Rashba effect, by modifying local inversion symmetry. In this presentation, we will illustrate some of our recent achievements on layered lead halide perovskites.

Mots-Clés: pressure, crystal structure

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*Intervenant

Pressure-induced local disorder and bandgap evolution in CsPbBr3

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Résumé

Halide perovskites exhibit remarkable optoelectronic properties that are strongly coupled to their lattice structure and dynamics. Hydrostatic pressure provides a powerful tool to probe and tune these structure–property relationships, often leading to significant changes in optical behavior such as bandgap shifts. However, the microscopic structural mechanisms underlying these optical changes remain incompletely understood, particularly the role of local disorder preceding pressure-induced amorphization.

In this work we investigate the pressure-dependent structural and optical evolution of the inorganic halide perovskite CsPbBr3 using synchrotron total X-ray scattering combined with reverse Monte Carlo (RMC) big-box modeling. While conventional diffraction indicates that long-range crystallographic order is preserved up to around 2 GPa, the pair distribution function (PDF) analysis reveals pronounced local structural distortions developing already within the orthorhombic phase. These include progressive displacement of Cs cations and increasing distortions of the PbBr6 octahedra.

By reconstructing atomistic configurations consistent with the total scattering data, RMC modeling provides direct insight into the evolution of octahedral bond angles and local structural disorder under compression. We find that the pressure dependence of the optical bandgap closely follows the evolution of octahedral tilting: up to 1 GPa, a reduction in tilting enhances orbital overlap within the Pb–Br framework, leading to bandgap narrowing, while at higher pressures the reappearance of tilting and increasing angular disorder cause the bandgap to widen.

Above 2 GPa the system undergoes partial amorphization, with significant disordering of Cs and Br, while the Pb sublattice remains preserved, allowing for structural recovery upon decompression.

Our results demonstrate that local structural disorder plays a central role in governing the

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*Intervenant

optical response of CsPbBr3 under pressure. Understanding how local structural distortions influence optoelectronic properties provides new insight into structure–property relationships in halide perovskites and may guide strategies to design materials with optimized functional properties.

Mots-Clés: High, Pressure, Structure–property relationships, X, ray total scattering

Collective Spectral Diffusion of Defect Luminescence in CH3NH3PbI3 Single Crystals

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Résumé

Many of the unique properties of halide perovskites are believed to be related to their soft, polar lattice. Understanding the interactions between defects, the lattice, and charge carriers requires further investigations at the microscale.
Single crystals exhibit very low defect densities and superior optoelectronic properties compared with polycrystalline thin films, (1,2) making them an ideal platform for studying the intrinsic properties of these materials.(3,4) At very low temperatures, defect states associated with energy levels within the band gap can be directly observed through their photoluminescence (PL).

Low-temperature PL spectroscopy of high-quality single crystals reveals ultra-sharp emission lines (_˜100 μeV at 4 K).(5) Detailed analysis of steady-state and time-resolved PL indicates that these lines can be assigned to donor–acceptor pairs (DAPs). Photoluminescence excitation spectroscopy further demonstrates an efficient excitation pathway for these defect states below the band gap.

The ultra-sharp emission lines exhibit significant temporal fluctuations in their emission energy, with amplitudes ranging from hundreds of μeV to several meV. Statistical analysis of spectral diffusion (SD) reveals a transition from Gaussian to Lorentzian statistics with increasing excitation power, attributed to photoinduced spectral jumps. Additionally, synchronicity is observed in the emission of multiple lines, suggesting coupling between an ensemble of defect states and slow, correlated lattice deformations.

These results provide new insights into the nature of defect states in halide perovskites and their interaction with the lattice.

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Mots-Clés: Halide Perovskite : Photophysics : Defects : Spectral diffusion

Semiconducting perovskites for the future of medical radiography: experimental characterization of charge-carrier transport properties through laser Time-of-Flight measurements

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Résumé

Recent studies have shed light on the attractive properties of metal halide perovskites for direct X-ray detection in medical imaging (1). Semiconducting perovskites can directly convert X-ray photons into electric signals, paving the way for combining higher sensitivity and better spatial resolution. Among them, CsPbBr3 is particularly studied (1,2), as its high atomic number allows good X-ray absorption. While CsPbBr3 performance is promising, its charge-carrier transport properties remain poorly understood. This work presents a preliminary study of the carriers mobilities through laser Time of Flight (ToF) measurements. Mobilities of both carriers can be extracted with ToF measurements, which probe the transport inside the bulk. With an above-bandgap energy laser, electron-hole pairs are generated, and one type of carriers can be collected on the opposite electrode by applying a high electric field. If, in theory, the interpretation of ToF data on ideal semiconductors is straightforward, photocurrent measurements conducted on 200-μm-thick polycrystalline layers of CsPbBr3 done by sublimation (3) revealed a cusp shape, for which a high injection regime is hypothesized (4,5,6). A high density of injected carriers leads to a deformed electric field in the material, which propagates with the drifting charge distribution (6). Considering the space charge perturbation induced by the high injection regime, charge carrier mobilities have been extracted from those signals, and they were evaluated at about for both carriers, in good agreement with literature data on perovskites (7). A study of the ToF photocurrent evolution over time revealed the degradation of the signal under DC bias, consistent with ionic migration leading to a screening of the electric field (8). This effect was reversed by switching bias polarity.

Mots-Clés: characterization, time of flight, mobility, CsPbBr3

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Probing Surface Chemistry of CsPbBr3 Nanocrystals with DNP-Enhanced Solid-State NMR at 30 K

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Abstract

CsPbBr3 and other halide perovskite nanocrystals have sparked significant interest due to their exceptional optical properties. However, their seemingly simple colloidal synthesis has proven challenging, primarily due to the soft ionic nature of their core and the lack of stability. Precise determination of the surface chemistry is essential for optimal ligand design to render these nanocrystals more stable. Solid-state NMR can be the ideal technique for this purpose as highly specific and detailed information about the interface can be obtained by selectively probing ligand and perovskite nuclei. The primary limitation of the solid-state NMR is low sensitivity, which can be alleviated through hyperpolarization techniques such as Dynamic Nuclear Polarization (DNP). However, polarizing halide perovskite nanocrystals is extremely challenging, especially on commercially available systems that operate at 100 K. The sensitivity limitations can be drastically overcome by optimizing sample preparation for DNP, together with operation at 20-30 K using home-built instrumentation that sustainably employs cryogenic helium. As a result, experimental times for high quality NMR spectra can be significantly reduced, by 2 to 3 orders of magnitude compared with previous studies. Enabled by this considerable improvement in sensitivity, I will demonstrate a solid-state NMR toolbox comprised of intricate experiments which are essential for unambiguous determination of the surface chemistry of CsPbBr3 nanocrystals, and have been previously impossible. In conjunction with DFT simulations and TEM studies, these experiments provide critical information allowing to elucidate the nanocrystal stabilization mechanism, such as (1) nanocrystal surface terminations, (2) dual mechanism of ligand binding involving substitution and adsorption, and (3) cooperative ligand binding.

Keywords: CsPbBr3, Nanocrystals, Surface Chemistry, NMR

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In situ monitoring of the Synthesis of Air-Stable Mixed-Valence Inorganic Gold Perovskite Thin Films via Aqua Regia Oxidation Process

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Résumé

Lead-free double perovskites are emerging as promising alternatives to conventional lead halide perovskites, addressing toxicity and stability concerns. Among these, mixed-valence gold halide perovskites (AAuX) offer near-infrared bandgaps and enhanced stability, yet their synthesis into continuous thin films remains challenging. Here, we report an innovative, low-temperature aqua regia oxidation process that enables the direct conversion of metallic gold thin films into continuous, polycrystalline gold halide perovskite layers. This method overcomes the nucleation limitations of conventional spin-coating techniques, producing high-quality CsAuAuCl films with tunable morphology and optoelectronic properties. Using **in situ optical spectroscopy (photoluminescence, Raman, and transmission)**, we monitor the real-time growth mechanism, revealing the interplay between nucleation, crystallization, and reaction kinetics. Structural (XRD, XPS) analyses confirm the phase purity and stability of the films. To further optimize the process, we explore replacing the chemical oxidizing agent with **electro-oxidation via the application of an electrical potential**, offering a more controlled and scalable route for thin film fabrication.

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Mots-Clés: Lead, free double perovskites, Aqua regia oxidation, In situ optical spectroscopy, Near, infrared perovskites, Thin film growth mechanism.

Finite Temperature Modelling of Mixed-valence Double Perovskite Cs2AuAuCl6

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Résumé

Halide double perovskites (HDPs) have emerged as promising alternatives to conventional perovskites, addressing challenges associated with structural instability and lead-induced toxicity. Among the HDPs, mixed-valence gold chloride Cs2Au1+Au3+Cl6, whereby a single metal cation exists in two oxidation states, has drawn particular interest owing to its unique structural and optoelectronic properties. However, the finite-temperature behavior of the electronic, optical, and phonon properties of this material is not well understood. Particularly, with increasing temperature, the absorption spectrum exhibits a redshift in the low-energy region and a blueshift in the high-energy region. Here, we investigate the temperature-dependent properties of Cs2Au1+Au3+Cl6 by combining first-principles density functional theory (DFT) with special displacement method (SDM) based calculations. We found that temperature-induced lattice expansion (LE) and electron-phonon coupling (EPC) impose opposing effects on the electronic structure of this material, such as, while the LE increases the bandgap, EPC reduces it at nearly the same rate (_˜0.5 meV/K). Therefore, the conventional approach of treating the two effects independently leads to a negligible or vanishing temperature dependence of the bandgap, highlighting the need for a more rigorous and coupled treatment of LE and EPC. Furthermore, the temperature-dependent phonon dispersion calculations suggest the presence of strong anharmonic effects in the material. Without anharmonicity, the Raman mode temperature evolution disagrees with experimental observations. From the electronic structure calculations, incorporating all three effects, we observed that the bandgap decreases with increasing temperature. Moreover, from spectral function calculations, the conduction band states are found to be significantly broadened at finite temperatures. This work, thereby, demonstrating the strong EPC and anharmonic effects in Cs2Au1+Au3+Cl6, highlights the importance of accurate treatment of temperature-induced effects in finite-temperature modelling of this exciting class of materials.

Mots-Clés: Perovskite, Photovoltaics, electron, phonon coupling, Anharmonicity

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Add, Mix, Heat, Repeat: Automated Combinatorial Synthesis of Hybrid Perovskite Materials

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Résumé

Theoretical and predictive chemistry signficantly outpace experimental chemistry, however, synthesis and experimentation are unavoidable bottlenecks in materials development. HiWAY-2-MAT (High-throughput combinatorial and autonomous pathways in solid state chemistry) is a multistage platform designed to rapidly produce libraries of solid-state materials to help accelerate materials screening. It consists of a robotic chemistry platform offering automated powder and liquid measurement and handling, heating and stirring units, and the capability of filtering materials directly into x-y grids for analysis. High throughput instrumentation is then used for materials analysis. For characterisation high-throughput XRD is currently operational, with fluorimetry planned in the mid 2026 period.

Hybrid alkali halogen perovskites (ABX, where A is an organic cation, B is an alkali metal cation, and X is a halogen) are an underexplored area of lead-free perovskite materials which are non-toxic, prepared from abundant elements, and show interesting luminescent properties. The high number of potential variations of A, B, and X which retain similar handling conditions, make their synthesis well-suited to the automated combinatorial approach offererd by the HiWAY-2-MAT platform.

In this work we discuss the requirements and considerations that must be taken into account when adapting perovskite synthesis reactions to automated platforms, and preliminary results obtained in the synthesis of the material libraries.

Mots-Clés: hybrid perovskite, automation, lead free, machine learning

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Beyond the Surface: Three-Dimensional Probing of Self-Assembled Monolayers in Perovskite Solar Cells

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Résumé

Self-assembled monolayers (SAMs) are widely employed to tune interfacial properties in perovskite solar cells (PSCs), yet have so far been regarded as strictly two-dimensional surface modifiers. Here, we uncover the three-dimensional nature of perfluorinated silanol-based SAMs applied onto perovskite films and their impact on both the photovoltaic performance and stability of PSCs. Using high-resolution three-dimensional nanoscale secondary ion mass spectrometry (NanoSIMS), which directly maps their lateral and vertical distribution, we reveal that these SAMs not only decorate the perovskite surface but also selectively penetrate and anchor at grain-boundary iodine-deficient regions within ∼100nm of the film. This dual surface-bulk passivation reshapes the defect landscape in perovskite thin films, yielding reduced non-radiative recombination, favorable interfacial energetics, enhanced photovoltaic performance, and increased environmental stability. Our findings reposition SAMs as volumetric chemical modifiers, rather than merely interface dipole layers, opening new opportunities for molecular-level engineering in perovskite optoelectronics.

Mots-Clés: Perovskite solar cells, Self, assembled monolayers, NanoSIMS, stability

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Broadband Emission in Low-Dimensional Hybrid Alkali Halide Perovskites

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Résumé

Chemists have recently focused on the preparation of lead-free hybrid metal halide perovskites for applica-tions in optoelectronics, aiming to mitigate toxicity while maintaining favorable photophysical properties. In most cases, the broadband emission of such materials has been attributed to self-trapped excitons (STEs). However, the family of hybrid alkali halide perovskites, in which lead metal ions are substituted by alkali metal ions, has been neglected. Herein, we report the low-dimensional hybrid alkali halide per-ovskite phosphor, ((pipH2)3I2)CsI5·H2O (pip = piperazine, C4N2H10), which exhibits orange-red emission and can be employed in phosphor-converted LEDs. Using a temperature-dependent emission-excitation matrix and power-dependent photoluminescence (PL) spectroscopic techniques, the photoemission of the 1D perovskite material is shown to originate from defect states related to an excess of iodine rather than the STEs, thereby evidencing the important role of defect states in broadband emission. Exploring this family of low-dimensional hybrid alkali halide perovskites could provide insight into the photolumines-cence mechanism and be a route to the discovery of numerous low-cost, non-toxic, and stable materials for optoelectronics.

Mots-Clés: New Low, dimensional Alkali Halide perovskite, Broad emission, pcLEDs, Density functional theory

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Collective effects in the photoemission of CsPbBr3 nanocrystals studies by time-resolved spectroscopy: temperature and fluence dependency

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Résumé

Halide perovskite materials are of particular interest for the development of several optoelectronic applications, including light-emitting devices (LEDs and lasers). This is due to their excellent optical properties, such as high absorption cross-section and high fluorescence quantum yield. Recently, superfluorescence (SF) in ordered nanocrystal superlattices was reported, generating a large interest in the community and rising several questions relative to the possibility to obtain coherent collective emission process in solid-state materials. Here we study the time-resolved photoluminescence of films of weakly confined CsPbBr3 nanocrystals with a picosecond streak camera, under various excitation fluences and temperatures (from 80 to 300 K). Giant oscillator strength effect is observed when decreasing the temperature, with the acceleration of the radiative lifetime. At very high excitation fluence, fast amplified spontaneous emission emerges (IRF limited to a few picoseconds), while exciton recombination dynamics are dominated by non-radiative Auger recombination (tens to hundreds of femtoseconds).

Mots-Clés: ultrafast exciton dynamics, time, resolved photoluminescence, CsPbBr3 nanocrystals

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Corrosion of Metals in Chloride/Bromide Environments: Towards Systematic Corrosion Studies in Halide Perovskite Cells

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Abstract

Corrosion is a significant challenge in halide perovskite systems, which, despite their exceptional photoconversion efficiencies, struggle with long-term stability. Perovskites are reactive materials capable of degrading metal electrodes, including those made with noble metals like gold. These interactions are influenced by light, heat, and the material's partial chemical transformations, which can either stabilize or exacerbate corrosion. This complexity poses major challenges for the durability of perovskite systems, making corrosion mechanisms a critical area of study.

We examine the known reactions between perovskites, metals, and transport layers, along with their impact on device durability. Although a few corrosion protection strategies have been proposed, they often fall short, reflecting a lack of comprehensive understanding of these reactions. A detailed investigation of perovskite chemistry and its interactions with other components is essential for developing effective protection strategies and provides the foundation for new approaches to mitigating corrosion.

As a first step, we investigate the electrochemical corrosion behavior of key electrode metals such as gold, alongside aluminum, copper, and silver in chloride and bromide solutions containing relevant cations (e.g., Cs, methylammonium). Unexpected differences observed in open-circuit potential and polarization resistance measurements suggest the formation of (partially) passivating interfacial layers whose properties are strongly cation-dependent.

To elucidate the exact chemical nature of these interfaces, we correlate macroscopic electrochemical findings with direct microstructural characterizations. X-ray diffraction (XRD) and Raman spectroscopy are employed to identify specific crystalline corrosion products and metal-halide bonds. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) is used to characterize the electrode surfaces. Together, these results reveal how specific ions influence interfacial stability in halide-rich environments. Ultimately, these fundamental understandings provide crucial guidelines for the design, material selection, and fabrication of highly durable perovskite optoelectronic devices.

Keywords: Halide perovskites, Electrodes, Corrosion, Surface chemistry

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Élaboration et caractérisation de couches minces de pérovskites pour le développement de capteurs de gaz

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Résumé

Les pérovskites hybrides émergent comme des matériaux prometteurs pour le développement de capteurs de gaz de nouvelle génération. Grâce à leur forte mobilité des porteurs, à la sensibilité de leurs propriétés électroniques aux espèces adsorbées et leur synthèse basse température, ces matériaux offrent un fort potentiel pour la réalisation de dispositifs portables ou embarqués capables de suivre les variations spatio-temporelles des traceurs gazeux (O, NO, COV, etc.).

A l'ICMN, nos activités de recherche visent à explorer le potentiel des pérovskites hybrides pour la détection de gaz. Dans ce cadre, nous étudions les corrélations entre la microstructure des couches minces et leurs propriétés optiques et électroniques afin d'évaluer la faisabilité de leur utilisation dans ce type d'application. Des couches minces de pérovskite MAPbBr sont choisies en raison de leur stabilité améliorée. Elles sont synthétisées et déposées sur des différents substrats. L'utilisation d'un anti-solvant lors du dépôt permet de contrôler la cinétique de cristallisation et la morphologie des films.

Nous présenterons l'analyses des films minces les plus prometteurs, caractérisés par microscopie optique, microscopie à force atomique (AFM) spectroscopie Raman, mesures de photoluminescence stationnaire et résolue en temps ainsi que par spectroscopie photoélectronique à rayons X (XPS).

Mots-Clés: Pérovskites hybrides, Raman, Photoluminescence stationnaire, Capteur de gaz, Film mince

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Engineering Scalable and Stable Perovskite Solar Cells in Air via Printed Interlayers and Encapsulation

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Résumé

The development of scalable, high-performance, and stable perovskite solar cells (PSCs) is a critical step toward their practical implementation in clean energy technologies. In this work, we present an integrated study combining scalable device fabrication and advanced encapsulation strategies, based on two complementary investigations. First, we demonstrate fully blade-coated p–i–n perovskite solar cells processed entirely in air, incorporating a nanometer-thick bathocuproine (BCP) buffer layer deposited by blade coating. This approach enables the fabrication of efficient devices while remaining compatible with roll-to-roll manufacturing. The blade-coated BCP layer acts not only as an effective hole-blocking layer but also as a surface planarizer, reducing interfacial roughness and charge recombination. As a result, power conversion efficiencies approaching 15% were achieved on 0.5 cm^2 devices, with improved reproducibility and operational stability under ambient conditions. Building on this scalable architecture, we further investigate encapsulation strategies aimed at mitigating extrinsic degradation caused by oxygen, moisture, heat, and prolonged illumination. Acrylic- and epoxy-based adhesives were systematically evaluated for the encapsulation of blade-coated PSCs. Electrical performance, calcium tests, water immersion, and thermal aging under ISOS-D-2 conditions revealed that epoxy-based adhesives provide superior barrier properties and long-term thermal stability, preserving device functionality for thousands of hours. In contrast, acrylic encapsulants exhibited faster lateral permeation and performance losses under harsh environmental stress. Together, these results demonstrate a viable pathway toward industrially relevant perovskite solar cells, combining air-processed, scalable fabrication with robust encapsulation strategies. The integration of printed interlayers and optimized edge-sealing materials represents a significant step toward stable, flexible, and commercially viable perovskite photovoltaic technologies.

Mots-Clés: perovskite solar cells, scalable processing, blade coating

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Functional Carbazole Molecules as Potential SAM Charge-Transporting and Interfacial Materials for Perovskite Solar Cells

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Résumé

Perovskite solar cells (PSCs) are considered a highly promising next-generation photovoltaic technology owing to their high power conversion efficiencies, simple fabrication processes, and low production costs. Recently, self-assembled monolayer (SAM) molecules have attracted increasing attention as an effective strategy to improve device performance and enhance operational stability. In these systems, SAMs function not only as hole-transport layers but also as interfacial modifiers.

In this presentation, I report our initial results on the development of functional carbazole-based small molecules designed for application as SAM hole-transport layers (HTLs).

Keywords: Perovskite solar cells, self-assembled monolayer, hole-transport layer, interfacial modifier.

Mots-Clés: Perovskite solar cells, self, assembled monolayer, hole, transport layer, interfacial modifier

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High throughput screening of Lead-free Halide Double Perovskite thin layers grown by Close Space Sublimation (CSS)

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Résumé

Sustainable energies are one of the major current research fields, trying to solve both ecological and economical aspects of modern society challenges. Photovoltaic (PV) energy contributes more and more to World energy diversity because of its lower cost, modular and easy applications compared to other energy sources. While most of commercial solar cells are based on silicon semi-conductors' technologies, an emerging alternative opens a new perspective: Lead-based Halides Perovskites (APbX3). Even if the performances are competitive and could suit the economical aspect of the energetic transition, Lead toxicity isn't suited for the ecological and European legislation aspect. An emerging solution would be to explore the lead-free halide double perovskite family (DHPs) A2M(I)M(III)X6 (A = Cs, CH3NH3, CHN2H4 ;M(I) = Ag+, Na+, Au+, Cu+, K+, etc... ;M(III) = Bi3+, Sb3+, In3+, etc... ;X = Br, I, Cl) which offers a wide panel of chemical possibilities to tailor the material and optoelectrical properties. In order to address such a vast topic, the use of screening processes is imperative to test multiple composition in a reduced timeframe. Solution-based deposition processes are giving promising answers at laboratory scale but still lacks the industrial scalability. The solution developped uses a vapor deposition process: Close Space Sublimation (CSS) to identify, novel semiconducting materials that are susceptible to replace current PV semi-conductors with an easier transferable growth process. A custom CSS growth furnace will be designed and built at CEA Grenoble. This furnace will allow to screen large number of growth conditions (temperature, chemical composition) within one single experiment. This new furnace will be used to accelerate the optimization of thin layer deposition of DHPs such as Cs2AgBiBr6, as well as to screen new M(I) and M(III) metals. This study will allow to accelerate the discovery of promising lead-free sustainable PV materials.

Mots-Clés: Lead, free Halide Double Perovskite, Thin layer, CSS, Photovoltaic

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Improved Thermal Stability of Perovskite Solar Cells via Hole Transporting Materials Design

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Résumé

Perovskite solar cells (PSCs) have been considered as an undeniable candidate for next generation photovoltaic technology, eventually exceeding the power conversion efficiency (PCE) of silicon solar cells by achieving 27.0% of a certified record in 2025. While approaching to commercialization of PSCs on the basis of remarkable PCE values, PSCs still suffer from unstable long-term performance particularly at elevated temperature, which is frequently attributed to poor morphological stability of spiro-MeOTAD being generally used as hole transporting material (HTM) for n-i-p architecture. In this work, we explore the new HTMs employing a consistent bulky central core with varying functional groups with closely correlating opto-electrochemical properties and photovoltaic performance to understand the role of respective functional groups in designed HTMs. One of designed HTMs eventually demonstrated outstanding thermal stability by ensuring morphological stability though the related PCE was not remarkable. Nevertheless, we believe the content of this paper certainly has a feasible insight into designing new HTMs and will be of great interest for the broad understanding in terms of stability issue of PSCs.

Mots-Clés: Hole transporting material, thermal stability

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Interface Engineering in CsPbBr Nanocrystal Thin Films and Superlattices for Light-Emitting Devices

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Résumé

Cesium lead bromide (CsPbBr) nanocrystals are highly attractive quantum-dot emitters for light-emitting diode (LED) applications due to their narrow emission linewidth, high photoluminescence quantum yield, and excellent color purity. Despite these advantages, the performance and operational stability of CsPbBr nanocrystal LEDs remain strongly limited by interfacial effects within nanocrystal films and at device contacts.
My PhD research focuses on understanding and engineering interfaces in CsPbBr nanocrystal thin films, with the objective of improving charge injection, reducing non-radiative recombination, and enhancing long-term stability in LED devices. Particular attention is paid to surface ligand chemistry, ligand exchange strategies, and their impact on nanocrystal coupling, defect passivation, and film morphology. These interfacial parameters critically determine the balance between efficient charge transport and preservation of the quantum-confined optical properties.

Beyond LEDs, this work also explores the controlled three-dimensional assembly of CsPbBr nanocrystals into ordered superlattices as a platform to study collective electronic and optical effects arising from strong inter-nanocrystal coupling. Insights gained from these model systems are relevant not only for LEDs but also for emerging photovoltaic architectures, where interface-driven recombination and ion migration remain key challenges.
Overall, this research aims to establish clear structure–interface–property relationships in CsPbBr nanocrystal assemblies, enabling rational interface design for stable, high-performance optoelectronic devices.

Mots-Clés: Perovskite, CsPbBr, LED, quantum dots

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Interplay of the charged and neutral excitons in single perovskite quantum dots

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Résumé

Lead halide perovskite quantum dots (pQDs) have emerged as promising candidates for quantum light sources. They exhibit high photoluminescence efficiency, narrow emission linewidths, and emit single photons up to room temperature, with photon indistinguishability reaching up to 50% at cryogenic temperatures.

Notably, bright emission is maintained with relatively simple organic ligand passivation, despite the presence of charging processes. Yet, the impact of these charge fluctuations on photon emission dynamics remains poorly understood.
In this study, by using micro-photoluminescence experiments at cryogenic temperature, we investigate the interaction between the charged exciton and the neutral exciton in individual CsPbBr3 perovskite quantum dots. Power-dependent spectroscopy reveals the presence of both neutral and charged excitonic transition sin the emission spectrum. Time-resolved intensity traces show an anti-correlated behavior between exciton and trion states, with no simultaneous emission, as confirmed by second-order correlation measurements. Despite this switching, the two states exhibit comparable radiative quantum yields, and the sum of their contributions results in stable radiative emission.

To further characterize this switching, we conduct intensity correlation measurements over time scales ranging from 100 ps to several minutes. The analysis demonstrates characteristic transition times between exciton and trion states, providing insight into the charging and neutralization mechanisms governing the emission dynamics.

Ongoing work, supported by simulations based on a random population model, aims to clarify the microscopic origin of these charge dynamics and their possible connection to non-radiative and trapping processes.

Mots-Clés: Quantum Dots, Charge Fluctuation, Exciton, Trion dynamics, Single Particle Spectroscopy, Photoluminescence, Single Photon Source

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Mesure de la diffusion ionique et de l'évolution des phases secondaires dans CsPbBr3 par XRF en incidence rasante et XRD

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Résumé

Les pérovskites halogénées sont étudiées pour servir de détecteurs directs de rayons X pour la radiographie médicale de grande surface, pouvant surpasser les imageurs indirects actuels grâce à une meilleure résolution spatiale et un signal accru. Cependant, les effets de la migration ionique, notamment induite par la polarisation électrique, ainsi qu'un gain de photoconduction variable, sont des facteurs d'instabilité limitant leur fonctionnement.
Nous avons cherché à savoir si la migration ionique mène à une réorganisation structurale de la pérovskite.

Pour ce faire, nous avons réalisé une analyse de diffractométrie des rayons X *operando* sous polarisation électrique à l'aide d'un goniomètre également équipé d'un détecteur de fluorescence X, permettant l'étude simultanée de la migration ionique et de l'évolution des phases structurales en fonction du champ électrique appliqué à nos échantillons de ITO/CsPbBr3/Cr polycristallins.

Nous avons trouvé que des phases de CsBr, Cs4PbBr6 et CsPb2Br5 se sont formées près de la surface dans nos échantillons ayant subi une polarisation électrique pendant plusieurs dizaines d'heures. Nos expériences *operando* nous ont permis d'observer que la formation de ces phases, ainsi que la décomposition de CsPbBr3, sont corrélées aux changements du signe de la polarisation électrique de nos échantillons. De même, la migration des espèces de Cs, Br et Cr est corrélée au signe de la polarisation électrique.
Ainsi, nous avons mis en évidence une instabilité structurale aux interfaces de dispositifs à base de pérovskites halogénées due à la migration ionique causée par la polarisation électrique. La modification de ces interfaces pourrait avoir un lien avec l'apparition et l'instabilité du gain de photoconduction mesuré expérimentalement sous irradiation X. Ces résultats sont

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la conclusion de mon stage de master ; mes recherches actuelles en thèse concernent la compréhension des mécanismes du gain de photoconduction et son (ses) origine(s) dans les mêmes dispositifs à pérovskites halogénées.

Mots-Clés: XRD, XRF, migration ionique, ionic migration, phases, structure, bias, polarisation

Multifunctional Polymeric Materials for Perovskite Solar Cells

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Résumé

Multifunctional Polymeric Materials for Perovskite Solar Cells

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Abstract

Perovskite solar cells (PSCs) are among the most promising renewable energy technologies due to their high-power conversion efficiencies, low fabrication costs, and strong potential for a wide range of applications. The commercialization of PSCs has become increasingly realistic thanks to advances not only in perovskite photoactive materials, but also in charge transport layers, interfacial engineering, and processing technologies. In this context, polymers have emerged as multifunctional materials in the evolving architecture of PSCs, helping to address key challenges related to perovskite film formation, interface engineering, defect passivation, charge transport, and device stability. This work reports initial efforts toward the development of functional polymeric materials aimed at improving the performance and stability of perovskite solar cells.

Keywords: perovskite solar cells, polymers, multifunctional materials, charge transport.

Mots-Clés: perovskite solar cells, polymers, multifunctional materials, charge transport.

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Nanothermometry-Guided In Situ Decoding of Perovskite Solar Cell Degradation under Optical Stress

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Résumé

The operational instability of perovskite solar cells (PSCs) remains a key obstacle to their long-term performance and commercial deployment. While extensive efforts have been made to understand degradation mechanisms, direct probing of the buried interfaces, where critical degradation often initiates, has remained elusive. In this work, we introduce a new in situ methodology that harnesses the nanothermometric properties of embedded upconversion nanoparticles (UCNPs) placed at the buried perovskite/hole transport layer (HTL) interface. This approach allows, for the first time, real-time tracking of local interfacial temperature evolution during light-induced accelerated degradation, while simultaneously monitoring the device's optical and photovoltaic performance. Applied to PSCs with different perovskite compositions, this technique reveals non-trivial thermal signatures and distinct degradation regimes correlated with structural and optical changes observed via ex situ characterizations. The results uncover a dynamic interplay between heat accumulation, phase transformation, and material decomposition, offering insights into the spatiotemporal evolution of PSC degradation. Our work demonstrates that nanoscale thermal sensing at buried interfaces provides a powerful new diagnostic tool to elucidate the internal degradation pathways of perovskite solar cells.

Mots-Clés: Nanothermometry, perovskite solar cells, in situ degradation, buried interface, thermal evolution

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Poster 16

New scintillators based on 2D perovskite single-crystals for neutronic detection

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Résumé

Fast neutron detectors are essential for quantifying neutron flux in nuclear reactors, imaging the internal structure of large equipment, and detecting contraband or radioactive nuclear materials. However, no ideal technology currently enables efficient, accurate, and real-time detection of fast neutrons, which are high-energy, highly penetrating particles produced in nuclear fission reactions.
There is a growing interest in hybrid organic–inorganic halide perovskites, which exhibit scintillation under X-rays, gamma rays, and fast neutrons within a single material platform. In particular, two-dimensional (2D) perovskites contain both light elements, such as hydrogen in long organic cations, which are suitable for neutron detection, and heavy elements, such as lead, which enhance X- and gamma-ray absorption. Since neutrons are uncharged, their detection relies on elastic scattering with hydrogen nuclei, resulting in proton recoil. The emitted proton then interacts with the scintillator, exciting electronic states and ultimately leading to radiative recombination and light emission.

Additionally, 2D perovskites exhibit strong quantum and dielectric confinement, leading to large transition dipole moment, meaning a fast recombination of electron-hole pairs for high scintillation yield (> 20 000 photons/MeV) and fast decay time (_˜ns). These properties make them promising candidates for fast neutron detection and mix gamma/neutron discrimination.
The poster presents our approach to grow, from solution, centimeters-size single-crystal of 2D perovskite (PEA2PbBr4) and their optical characterizations under photoluminescence or radioluminescence.

Mots-Clés: 2D perovskites, single crystal, scintillator, neutrons

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Optimized LARP synthesis of CsPbBr3 perovskite quantum dots for single nanocrystal spectroscopy

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Résumé

Colloidal perovskite quantum dots (pQDs) are highly promising quantum light emitters. To date, investigations at the single-pQD scale have predominantly relied on the hot-injection synthesis method, which is performed under an inert atmosphere and at high temperature. In contrast, the ligand-assisted reprecipitation (LARP) method is carried out under ambient atmosphere and at room temperature, making it a more accessible alternative. However, LARP is typically employed for the synthesis of pQDs intended for ensemble studies rather than for single-nanocrystal investigations (1). In this work, we report the optimization of the LARP method to synthesize pQDs suitable for individual spectral studies. Monodispersity was improved by introducing amines (PPA) during the synthesis (2), while ligand-tailoring was implemented through the incorporation of DDAB to better protect the pQDs. The nanocrystals obtained using this improved protocol exhibit high crystalline quality, as confirmed by high-resolution transmission electron microscopy (HRTEM) measurements, as well as high monodispersity evidenced by both TEM imaging and spectral measurements. Furthermore, they demonstrate single-photon emission with a second-order autocorrelation value of g(2)(0)=0.01, reaching the standards typically achieved with hot-injection-synthesized pQDs. In addition, the ease with which DDAB can be incorporated as a surface ligand is encouraging for future ligand-engineering studies. Also, functionalization of the terminal group of the amine molecules enables the fabrication of superstructures in solution, with

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varying shapes (3). Overall, this optimized LARP method constitutes a versatile approach that enables a broad range of optical investigations on pQDs.

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Mots-Clés: Perovskite, Quantum Dots, Ligand Assisted Reprecipitation Synthesis, Single Particle Spectroscopy, Photoluminescence, Single Photon Source

PRISM: Benchmarking Halide Perovskite Single Crystals for X- and Gamma-Ray Spectrometric Imaging

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Résumé

High-resolution X- and gamma-ray spectrometry (20 keV–1 MeV) currently relies on CdZn Te single crystals for applications in nuclear monitoring, astrophysics, and medical imaging. Despite their high performance, these materials face challenges related to production costs and the difficulty of growing large-volume crystals. Halide perovskites, such as all-inorganic CsPbBr, have recently emerged as alternative semiconductors. They offer high stopping power and favorable charge transport properties, with the added advantage versatile growth methods ranging from Bridgman (< 600 ◦C) to solution-based processes (< 100 ◦C) . However, most reported studies focus on isolated single-pixel detectors, making it difficult to assess their true potential for complex imaging systems.

The PRISM project (PeRovskIte gamma-Ray SpectroMetric imager) is a collaborative CEA initiative bringing together multidisciplinary expertise across diverse fields, including medical imaging, security, and astrophysics. The aim is to bridge the gap between material discovery and functional imaging systems. The project focuses on assessing the performance of commercially available halide perovskite single crystals against established CdTe references. A core objective is the development of a dedicated, reproducible characterisation platform to measure leakage current, charge carrier transport properties, and spectrometric response under identical experimental conditions. This approach is specifically designed to address performance dispersion and statistical reliability, moving beyond isolated best-case results to evaluate the reproducibility and temporal stability of these materials. The crystals will also be integrated into multi-pixel imaging architectures in order to evaluate their suitability for application-specific spectrometric imaging systems. The project will thus provide the first systematic benchmark of halide perovskite single crystals for spectrometric imaging applications.

Mots-Clés: Gamma, Ray, Single Crystal, Detector

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Random Lasing in All-Inorganic Perovskite - CsPbBr3 Metasurface

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Résumé

Random lasers represent a unique class of coherent light sources where optical feedback is generated by multiple scattering rather than by a conventional well-defined cavity. Halide perovskites, owing to their crystalline nature where grain boundaries act as natural scattering centers, have emerged as promising candidates for random lasing (RL) (1). In this work, we combine stable all-inorganic CsPbBr3 perovskites (2) with subwavelength metasurfaces fabricated by pressure- and temperature-assisted recrystallization using a patterned mold (3) to achieve directional control over RL emission (4). While unpatterned perovskite regions exhibit only amplified spontaneous emission, the engineered structural disorder within the metasurface significantly enhances scattering, enabling coherent feedback. The transition to the lasing regime is validated through single-shot spectral analysis, identifying characteristic Lévy-like intensity fluctuations and replica symmetry breaking (RSB) (5). A clear lasing threshold of approximately 17 μJ.mm^2 is observed. These findings highlight the potential of perovskite-based metasurfaces as a scalable and promising platform for integrated photonic light sources.

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Mots-Clés: Random lasing, All, inorganic perovskite (AIP), Metasurface, Nanoimprint, Replica symmetry breaking

Scalable pulsed laser deposition of CsPbI3 for perovskite-on-silicon tandem solar cells

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Résumé

Tandem solar cells are a promising architecture to increase the performance of silicon solar cells. Perovskite-on-silicon tandem solar cells reached 34,85 % of Power Conversion Efficiency (PCE) in 2024 on small areas (1), higher than the experimental limit of _˜27 % for single-junction silicon cells (1). In order to transfer this technology to the industry, the perovskite layer should be deposited on state-of-the-art silicon solar cells. This raises the issues of deposition on large areas, as well as on micron-scale pyramidal textured surface, which improves light trapping. Thus, we have developed Pulsed Laser Deposition (PLD) process, which allows conformal and uniform deposition of perovskite up to 707 cm^2, along with high deposition speed. CsPbI3 was chosen for its simple composition and for its bandgap of 1,7-1,73 eV, which is very close to the 1,7 eV optimal gap for a top cell on a silicon bottom cell. Currently, we are optimizing the perovskite phase through annealing/quenching and compositional engineering, as well as adjusting the PLD growth parameters. Integrations in perovskite single-junction cells and material characterizations are currently underway. Subsequently, we will move to the deposition on textured silicon bottom cells for integration in the tandem architecture. Afterwards, we will investigate the influence of the other layers' deposition methods, and the impact of passivation layers and intrinsic encapsulation, in order to design an integration process for achieving high performance and stable CsPbI3 on silicon tandem solar cells. (1) National Renewable Energy Laboratory, 2026.

Mots-Clés: CsPbI3, tandem, solar cells, inorganic perovskite, scalability, PLD, pulsed laser deposition

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Semiempirical DFTB Approaches for 3D and 2D Perovskites and Their Heterostructures

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Résumé

Understanding the physical properties of perovskite heterostructures is of significant interest for advanced optoelectronic and photovoltaic applications (1,2). In particular, band alignment predictions determine the relative positions of the band edges at an interface, enabling classification of the alignment type and assessment of carrier confinement, charge transfer, and transport properties (2-5). Density Functional Tight Binding (DFTB), a semiempirical method derived from Density Functional Theory (DFT), provides a computationally efficient framework for simulating large-scale periodic and nonperiodic systems. Previous studies have established optimized DFTB parameter sets for lead-iodide and lead-bromide perovskites (6, 7). In this work, we first outline the fundamental framework of DFTB, including its theoretical background and parameterization techniques. As several approaches have been developed within DFT to determine band alignment at heterointerfaces, we examine their transferability to the DFTB framework for 2D/3D lead-halide perovskite heterostructures. For transferable approaches, performance is benchmarked against DFT reference calculations by comparing band offsets to evaluate the accuracy and limitations of band alignment predictions within DFTB.

DFT and DFTB calculations were performed at FOTON Institute, and the work was granted access to the HPC resources of TGCC/CINES under the allocation A0160911434 and A0180911434 made by GENCI.

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Mots-Clés: Semiempirical, DFTB, Perovskites, Heterostructures, 2D/3D, Band alignment, DFT

Study of CsPbBr3 color conversion layers fabricated by PLD for color conversion in microLED displays

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Abstract

The fabrication of high-quality microdisplays for augmented reality has been shown to be challenging, mainly because this application requires small and bright Red, Green and Blue pixels. We propose to use a color conversion approach using blue microLEDs as light emitters and inorganic halide perovskite (IHP) thin films as color converters for green and red-light emission from blue light. IHP's have specific properties making them suitable candidates for this application as they are highly absorbent (≥ 4×10ˆ4 cmˆ{-1}), which allows for the use of thin films (< 1 μm), and could be highly stable thanks to its inorganic composition. In this work, we use the Pulsed Laser Deposition (PLD) method, which allows for the fast fabrication of wafer-scale IHP layers (Parrat, 2025). Here, the impact of the deposition temperature of CsPbBr3 deposited by PLD was studied, followed by different optical characterizations. This parameter has an impact on the film's morphology as well as how it evolves in time (over 4000h stored in air): the film's morphology deposited at high temperatures is more stable. This is also reflected on the optical performances of the film: the photoluminescence (PL) intensity is 70 times higher for the sample deposited at higher temperature. We have previously achieved a blue to green color conversion efficiency PLQY_{ext} of 48 % (with an estimated PLQY_{int} of 89 %) using this deposition method (Parrat, 2025). The current process used has shown to be repeatable with a PLQY_{ext} of 13 % (PLQY_{int} = 62 %), stable under illumination. The stability under continuous illumination has been tested for different excitation densities at 375 nm during 15 minutes, from 0.4 to 2260 W/cmˆ2 (extreme condition: ≥ 200 times higher than brightness estimated for AR). The results are promising, as the film is relatively stable for the first 15 minutes of illumination, even for higher excitation densities.

Keywords: CsPbBr3, Pulsed Laser Deposition, inorganic perovskite, Color Conversion Layers, stability

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Unveiling Clusteroluminescence in a Two-Dimensional Organic-Inorganic Hybrid Perovskite for Tunable Optical Properties

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Résumé

Low-dimensional organic-inorganic hybrid materials (OIHM) have garnered significant attention due to their versatile structural and photophysical characteristics. They hold promise for various optoelectronic applications, including the development of single-component white-light-emitting diodes. In this work, we report an unprecedented two-dimensional (2D) lead-chloride perovskite structure (TET)2(Pb4Cl16)1. Within this compound, saturated organic molecules surround inorganic layers, formed by bridging between clusters with a non-specific orientation. Under UV-visible excitation, the hybrid material exhibits a broadband white-light emission spanning the visible spectrum, excitation-dependent tunable luminescence and notably displays a green afterglow visible to the naked eye. A comparative optical analysis between the hybrid material and its corresponding organic salt was performed to elucidate the origin of these optical properties. It is revealed that clusteroluminescence plays a key role in the emission process, highlighting the significant contribution of the saturated organic molecules to the optical properties, despite their role often being overlooked

Mots-Clés: Organic Inorganic hybrid perovskites, Structure properties correlation, Clusteroluminescence

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*Intervenant