

Book of Abstracts

Online HOPE-PV 2020: Online School on Hybrid, Organic and Perovskite Photovoltaics
3rd - 5th November · 2020



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**School on Hybrid, Organic and Perovskite Photovoltaics (HOPE-PV20)
3rd to 5th November 2020**

Conference Chairs

Sergey M. Aldoshin, Jovana Milic, Keith Stevenson and Pavel Troshin

Tutorials	
Michael Graetzel	Ecole Polytechnique Federale de Lausanne
Artem Bakulin	Imperial College London
Juan Bisquert	Universitat Jaume I, Institute of Advanced Materials (INAM)
Christoph Brabec	Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
Francesca Brunetti	University of Rome (Tor Vergata)
Emmanuel Kymakis	Hellenic Mediterranean University
Monica Lira-Cantu	Catalan Institute of Nanoscience and Nanotechnology (ICN2)
Luigi Martiradonna	Nature Materials
Jovana Milic	University of Fribourg, Adolphe Merkle Institute
Sergei Ponomarenko	Enikolopov Institute of Synthetic Polymeric Materials of the Russian Academy of Sciences
Invited Speakers	
Sergey A. Adonin	Russian Academy of Sciences RAS · Nikolaev Institute of Inorganic Chemistry
QinYe Bao	East China Normal University
Vida Engmann	University of Southern Denmark, SDU NanoSYD, Mads Clausen Institute
Shijing Sun	Massachusetts Institute of Technology (MIT)
Alexey Tarasov	Lomonosov Moscow State University



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TUTORIALS

The Genesis and Rise of Perovskite Solar Cells

Graetzel, Michael *^a

a Ecole Polytechnique Federale de Lausanne (EPFL) (CH)

Over the last 10 years perovskite solar cells (PSCs) have emerged as credible contenders to conventional p-n junction photovoltaics. Their certified power conversion efficiency currently attains 25.5 %, exceeding that of the market leader polycrystalline silicon. The lecture will present the genesis and recent evolution of this new photovoltaic which has already produced over 15'000 scientific publications. I shall discuss their operational principles current performance and challenges that still need to be met to implement PSCs on a large commercial scale. PSCs can produce high photovoltages rendering them attractive for applications in tandem cells e.g. with silicon and for the generation of fuels from sunlight. Examples are the solar generation of hydrogen from water and the reduction of CO₂ mimicking natural photosynthesis.

Ultrafast Spectroscopy for Organic Photovoltaics

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One of the key areas of study in organic photovoltaics is the development of so-called 'nonfullerene acceptors' (NFAs), which enjoy several benefits over older, fullerene-based acceptors, including: low open circuit voltage losses, low cost, high absorptivity, and broad tuneability. Recent reports demonstrated conversion efficiencies up to 17% in donor acceptor blends of conjugated polymers and 'small' electron accepting molecules. However, these advantages come at the expense of light harvesting efficiency. In order to understand the processes underlying this remarkable efficiency, ultrafast spectroscopy methods are used.

In this tutorial I will introduce transient absorption (TA) spectroscopy - method most commonly used for time-resolved characterisation of photochemistry of organic and hybrid optoelectronic systems. I will demonstrate the typical experimental results as well as most commonly used approaches to the analysis and modelling spectroscopic data. I will show how TA can be applied to elucidate complex photophysics of NFA OPVs.

Fundamental Concepts of Photovoltaics and Operation of Devices for Solar Energy Conversion

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The research on advanced energy conversion devices as solar cells has evolved been intense in the last two decades. A broad landscape of candidate materials and devices were discovered and systematically studied and reported for effective solar energy conversion and utilization. New concepts emerged forming and a rather powerful picture embracing the mechanisms and limitation to efficiencies of very different broad types of devices has emerged from many discussions and sometimes also as well as from conceptual clashes. This talk is based on the book *Physics of Solar Energy Conversion* that introduces the main physico-chemical principles that govern the operation of energy devices for energy conversion and storage, with a detailed view of the principles of solar energy conversion using advanced materials. The talk is focused on the fundamental description of photovoltaic operation, mainly on new technologies from organics to metal halide perovskites. We explain the basic properties of interaction of a semiconductor with light, the physical properties controlling the production of current and voltage, the diode model with selective contacts, and the factors that control the energy conversion efficiency of the solar cell devices.

AMANDA - Line 1: Can AI Guided High throughput Device Engineering Resolve Long Time Challenges in Solution Processed Photovoltaics?

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Evaluating the potential of organic photovoltaics materials and devices for industrial viability is a multi-dimensional large parameter space exploration. Manual experimentation is extremely limited in throughput and reproducibility. Automated platforms for fabricating and characterizing complete functional devices can accelerate experimentation speed within tight processing parameter variations. Here we demonstrate a multi-target evaluation of organic and perovskite photovoltaic materials in full device level with the automated platform AMANDA Line 1 combined with Gaussian process regression-based data evaluation. Around 100 processing variations are screened within 70 hours which yield a reliable evaluation output in terms of efficiency and photostability. The unprecedented quality of the data coming from the AMANDA platform allow building correlation models by AI methods like Gaussian Parameter Regression (GPR). Already



several hundred samples allowed to research for hidden parameter correlations revealing structure – property correlations. One surprising correlation established a direct link between the absorption spectrum of a semiconductor composite and the performance and lifetime of a photovoltaic device. Such correlations have been previously searched for by highly complex experiments, including microstructure investigations on the synchrotron, but haven't passed the level of qualitative predictions. With AMANDA we have been able to build a quantitative correlation based on simple absorption spectroscopy. The implications of this research concept on the long time challenges in emerging photovoltaics will be discussed in the outlook of the talk.

Printable and flexible solar cells and energy storage systems: opportunities and challenges

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Printed new generation solar cells and energy storage systems are becoming more and more attractive thanks to the possibility of replacing conventional energy sources, reducing CO₂-emission and preventing the risk of global warming. On the other, thanks to the possibility of being generally processed at low temperature, they can be realized on lightweight and bendable substrates suitable for various applications, like transportable electronic chargers, flexible displays, biomedical devices, conformable sensors, and wearable electronic textiles. Among all the conventional and new-generation photovoltaic technologies, organic–inorganic metal halide perovskite solar cells (PSCs) exhibit appealing benefits that include high efficiency of up to 25.5%, low-temperature fabrication and solution-processability, which makes this technology compatible with most flexible substrates. On the other hands, for flexible storage technologies, supercapacitors are becoming the preferred technology when high capacitance and power delivery are required.

For the two type of devices, an important step in the direction of moving from lab to fab, is the scaling up of the printing techniques to manufacture large area devices. This aspect ideally should involve the use of green materials, the development of an in-line roll to roll process where all the layer are printed, with low waste of inks and highly reproducible. In this lecture, the state of the art for PSC and supercapacitors printed on flexible substrates will be reported highlighting the technological challenges to be faced when scaling up the device size, the possible solutions and the opportunities in terms of possible future applications given by these devices.



2D interfacial engineering for perovskite PVs: from small devices to solar systems

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The development of perovskite photovoltaics has matured to a point of industry-scale production; however, their operational long-term stability still remains the main obstacle impeding their direct commercialization. Remarkably, several approaches were undertaken with various degree of success to assess this issue, ranging from encapsulation, control over photoconversion process and selection of appropriate materials for effective charge extraction and collection. Among the plethora of possibilities, engineering solution processable materials with reduced dimensionality, such as graphene and related 2D materials (GRMs), appears to be a very promising approach, since the GRMs introduces minimal perturbation into the system and concurrently their intrinsic advantageous properties are positively reflected mainly on the device stability and incidentally, on performance. In principle, GRMs act simultaneously as barriers shielding the cell from moisture ingress/ion migration and energy alignment tool promoting efficient charge transfer.

In this talk, I will summarize our recent activities on the realization of highly efficient and stable perovskite solar cells and modules. I will give an insight on how the hierarchical placement of GRMs in all the perovskite device can tune the transport layers work-function, passivate the interface/surface traps and most importantly protect the interfaces, resulting in a simultaneously improvement of the triangle of performance, stability and scalability of the perovskite PVs. Furthermore, I will discuss the implementation of a Solar Farm consisting of GRMs-based PSCs modules, which reveals the strong impact of GRMs in the industrialization of this technology. The latter is a pivotal step toward successful and eventual large-area device fabrication and assembly into PV panels. I will also directly correlate the outdoor stability measurements of the PV modules with environmental parameters, while at the same time, benchmark their PV outdoor performance against commercial PV panels installed at the same site.

Metal Oxides for Highly Efficient and Stable Halide Perovskite Solar Cells

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Halide perovskite solar cells (PSCs) have emerged as a competitive photovoltaic technology with power conversion efficiencies (PCEs) surpassing the 23 % mark. One of the main bottlenecks of the technology is their long-term stability. Understanding the different degradation mechanisms of the constituent materials, as well as interface instabilities, is of crucial importance for commercialization. Semiconductor oxides (SO)

constitute a fundamental part of highly efficient PSCs. Electron transport semiconductor oxides, like TiO_2 , are characterized by an oxygen vacancy (O_{vac})-mediated conductivity caused by a deviation in stoichiometry, the presence of impurities, or both. In oxygen-containing atmospheres, and especially under UV light, holes generated at the nonstoichiometric oxide surface react with the oxygen adsorbed at an O_{vac} increasing charge recombination and degradation of the solar cell. Different methods have been employed to passivate or eliminate these O_{vac} . For example, the application of organic interfacial modifiers with anchoring groups specifically selected to bond with oxides, or the application of less reactive SnO_2 which results in less hygroscopicity, fewer O_{vac} at its surface, and less UV-damage. Another possibility is the application of a coating of secondary oxides, like Al_2O_3 , applied to suppress surface defects, avoid interfacial recombination, and enhance device stability. A less-explored option is the application of complex oxides with singular properties, such as ferroelectric, multiferroic, magnetic and similar.

In this talk, we report our most recent studies on the stability of perovskite solar cells by the application of metal oxides (binary, doped and complex oxides) applied as transport layers in Halide Perovskite Solar Cells. We also show the effect of the functionalization of the halide perovskite and the oxide layer applying simple organic molecules where the final PSC shows no degradation for up to 1000 h under continuous irradiation at 1 sun.

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An Insider's view on Nature Materials

Martiradonna, Luigi *^a

a Nature Materials

Nature Materials publishes cutting-edge research from all areas of materials science and engineering, offering authors high visibility to their work and helping developing a common identity among materials scientists. A team of full-time, professional editors selects and commissions articles that have the best chances to appeal to the journal's broad audience. In this talk I will provide an overview of the Nature family of journals, explaining their differences, similarities and relationship. I will also explain the process of a manuscript after submission to Nature Materials, and discuss the directions explored by our journals to provide great service to our authors.

Templating Hybrid Perovskites

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Future Approaches to Organic Photovoltaics

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INVITED SPEAKERS

Beyond Lead: Halide Complexes of 15 and 16 Group Elements, their Polyhalide Derivatives and their Use in Materials Design

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While Pb(II) halometalates are being very intensively investigated in the course of photovoltaic devices design, related derivatives of neighboring elements – bismuth, antimony and tellurium – remain significantly less considered in this area. Hereby, we present our recent achievements in synthetic chemistry of Bi(III), Sb(III) and Te(IV) halometalates and their polyhalide hybrids, as well as in their utilization in creation of solar cells and photodetectors.

This project was performed in close collaboration with Prof. Pavel A. Troshin (Skoltech, Russia).

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Interfacial Electronic Structures in Perovskite Solar Cells

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Degradation and Stabilization of Organic Solar Cells

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This lecture will focus on the degradation of organic solar cell devices. It will give an overview over the main degradation processes which occur under standard working conditions, and lead to decay of device performance as measured in stability testing lifetime setups according to ISOS protocols. Understanding of photooxidative degradation of the active layers will be given special attention, with an outlook on the stabilization strategies. Additive-assisted stabilization will be elaborated in detail, with up to date

examples from our group on the use of biomimetic singlet oxygen and fullerene triplet quenchers ^{1,2}, as well as from other groups reporting on the use of antioxidants, radical scavengers, UV absorbers, and similar, for stabilization of organic and perovskite solar cell devices ³.

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Data-driven Discovery in the Search for Stable Perovskite Photoabsorbers

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The environmental instability of organic-inorganic perovskite materials limits their usage in photovoltaics. we demonstrate a physics-constrained sequential learning framework to subsequently identify the most stable alloyed organic-inorganic perovskites. Compositional engineering is to date one of the most effective methods to improve perovskites' stability in the presence of heat, humidity and light without sacrificing optoelectronic performance. This fact has led to intensive research within combinatorial spaces such as $A_xB_yC_{1-x-y}Pb(I_zBr_{1-z})_3$. However, only a small fraction of this compositional space has been experimentally explored, in part due to the prohibitively expensive brute force synthesis. In this talk I will discuss our recent progress developing data-driven approaches that allow us to experimentally explore vast materials spaces in a resource-efficient fashion. We fuse data from high-throughput degradation tests and first-principle calculations into an end-to-end Bayesian optimisation algorithm to guide the optimization among multi-cation perovskites. By sampling just 1.8% of the discretized $Cs_xMA_yFA_{1-x-y}PbI_3$ (MA = methylammonium, FA = formamidinium) compositional space, multi-cation perovskites centred at $Cs_{0.17}MA_{0.03}FA_{0.80}PbI_3$ are identified showing minimal optical

change under elevated temperature, moisture, and illumination. Exemplified by this data fusion approach, I will discuss pathways towards autonomous perovskite discovery, where high-throughput experimentation and machine-learning techniques are combined to accelerate the search for stable perovskites in order to resolve the reliability challenge in the state-of-the-art perovskite solar cells.

New features of perovskite processing with Reactive Polyiodide Melts

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Perovskite solar cells are one of the fastest growing classes of photovoltaic devices overcoming record efficiencies for silicon solar cells and reaching power conversion efficiencies of 25.5%. While the solution techniques remain the most common approach for the fabrication of perovskite films, there is a difficulty with their scalability. Recently, a completely new approach for fabrication of large-scale perovskite films has been developed based on liquid polyiodide melts. The reactive polyiodide melts (RPM) are liquid polyiodides which can be readily prepared by mixing powders of I₂ with organic iodides such as MAI and FAI or a mixture thereof¹. The reaction proceeds instantly at room temperature and results in a highly-viscous liquid.

Based on the interaction of RPMs with metallic lead, high-quality perovskite films with various compositions were obtained according to the following reaction: $AX_3 + Pb \rightarrow APbX_3$ (A = MA, FA, Cs; X = I, Br). Thus, RPM opened up a new formation strategy of hybrid lead halide perovskites using the polyiodide-based method. Due to its unique composition the RPM acts simultaneously as a liquid medium and a highly reactive precursor that swiftly converts metallic lead into perovskite. Using this novel approach we fabricated high-quality polycrystalline perovskite films with micron-size grains with power conversion efficiency (PCE) of over 17%. The modules with 2.45 cm² active area showed PCE exceeding 14.2% with great uniformity of the perovskite layer over the large area. In addition, we demonstrated applicability of this method for the fabrication of highly uniform perovskite films with micron-size grains over large substrates of 10x10 cm² and 20x30 cm², including flexible supports.²

Moreover, the RPMs have been recently found to be also a highly corrosive decomposition product which forms under sunlight and cause degradation of perovskite solar cells components, including spiro-MeOTAD and gold electrode^{3,4}.

In the present study, we thoroughly investigated chemical and physical properties as well as phase equilibriums in the polyiodide systems and revealed the outstanding potential of the polyiodide melts for the improvement of the processing of hybrid perovskites.⁵

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Acknowledgments:

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CONTRIBUTED TALKS

ID: 003 Unravelling the Material Composition Effects on the Gamma Ray Stability of Lead Halide Perovskite Solar Cells: MAPbI₃ breaks the records

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Our joint experimental-theoretical work examined a variety of perovskites as gamma absorbers including MAPbI₃, MAPbBr₃, Cs_{0.15}FA_{0.85}PbI₃, Cs_{0.1}MA_{0.15}FA_{0.75}PbI₃, CsPbI₃, and CsPbBr₃. It was shown that the stability of the materials under gamma irradiation varies greatly among the materials. In particular, solar cells based on the MAPbI₃ were found to be the most resistant to gamma rays. This was explained by the defects formed in the materials undergoing rapid self-healing due to the dynamic behavior of this system. Fully-inorganic as well as mixed cation perovskite formulations did not deliver comparable stability due to the special gas-phase chemistry analyzed with ab initio

calculations, which occurs in MAPbI₃ but does not in other perovskites. This unique radiation-stability means that MAPI, while quite an unstable material in terrestrial conditions, is highly promising in space applications.

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ID: 008 Improving Operational Stability of Perovskite Solar Cells using ZnO Electron Transport Layer

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Low operational stability of perovskite solar cells represents a major obstacle for the practical implementation of this technology. In that context, ZnO may be considered as a promising electron transport material with suppressed oxidizing and photocatalytic activity as compared to SnO₂ or TiO₂. However, the first studies revealed the chemical instability of the interface formed between the lead halide perovskites and zinc oxide, whereas the underlying reasons are still under active debates. Still, the interfacial instability issues made ZnO a largely overlooked electron transport material despite its excellent optoelectronic properties.

In this talk, we present findings outlining the factors affecting the stability of the perovskite cells using ZnO electron transport layer (ETL) material. We found that the perovskite precursor chemistry plays a key role in the stabilization of the cells with this electron-transport layer. We show that, while using specific absorber and precursor formulations, the solar cells using ZnO demonstrate much superior operational stability compared to the devices that utilize SnO₂ or TiO₂ ETLs.

To further increase the lifetime of the perovskite solar cells using ZnO ETL, we developed a novel approach to the zinc oxide surface modification with methylammonium iodide that suppresses interfacial reactions with the adjacent perovskite absorber layer. The application of Cs_{0.12}[HC(NH₂)₂]_{0.88}PbI₃ as absorber material in devices with the modified ZnO electron transport layer resulted in 82% retention of the initial efficiency after aging for 2100 hours at 50 mW cm⁻² and 65°C. We attribute the revealed stabilization effect of

the methylammonium iodide treatment to passivation of the reactive ZnO surface and inhibiting the parasitic interfacial chemistry leading to the lead iodide formation.

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ID: 011 'Just Vibing': Coupled Organic and Inorganic Sublattices in Organohalide Perovskite Solar Cells

Gallop, Nathaniel P.^a; Maslennikov, Dmitry R.^a; Goetz, Katelyn^b; Sung, Woongmo^c; Nihonyanagi, Satoshi^c; Tahara, Tahei^c; Vaynzof, Yana^b; Bakulin, Artem A.*^a.

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Since their first use as photovoltaic absorbers in 2009, metal halide perovskites (MHPs) have proven to be among the most promising of the so-called 3rd generation photovoltaic technologies, owing to their superlative photovoltaic efficiencies, broad tuneability, and low production costs. For this reason, they have attracted considerable research attention, with over separate 13,000 papers published about them over the past 10 years¹. Despite this herculean effort however, there are still many things about MHPs that we do not yet entirely understand. Their soft nature and dynamic disorder—which arises in part from the interplay between the organic and inorganic sublattices that together comprise the material—makes reaching a comprehensive understanding of their dynamical behaviour very difficult². In particular, the degree to which the dynamics of the organic and inorganic sub-lattices are coupled to one and other—and this significance of this effect on the optoelectronic properties of MHPs—has generated considerable controversy within the literature, with researchers coming to conflicting conclusions about the nature and extent of the coupling^{3,4}. This is exacerbated by the relative dearth of conventional experimental techniques able to achieve the high sensitivities, selectivities, and time resolution needed to understand this effect.

To this end, in this talk I will discuss our development of a novel spectroscopic technique, which we term Photocurrent Detected Vibrationally Promoted Electronic Resonance (PC/VIPER) spectroscopy. This technique combines the so-called VIPER pulse sequence—first conceived as an extension to 2D-EXSY experiments⁵—with a highly sensitive interferometric photocurrent detection scheme, enabling us to both spectrally and temporally resolve the effect of vibrational transitions of the electronic properties of the organohalide perovskite FAPbBr₃, along with its all-inorganic counterpart CsPbBr₃. We find that stimulation of the C=N stretching mode of the formamidinium ion weakly modulates the bandgap of FAPbBr₃, with this effect being entirely absent in all-inorganic



CsPbBr₃. Through comparison with previously published 2DIR and DFT results, we rationalize this modulation as resulting from a weak coupling between the organic and inorganic sublattices, which distorts the inorganic lattice sufficiently to alter the bandgap. We conclude that, whilst the overall effect is weak, A-site cation dynamics cannot be entirely discounted when considering the optoelectronic behavior of certain organohalide perovskites.

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ID: 012 Exploring the radiation stability of perovskite solar cells

Boldyreva, Aleksandra * ^a; Frolova, Lyubov ^b; Zhidkov, Ivan ^d; Kurmaev, Ernst ^d; Gutsev, Lavrenty ^b; Aldoshin, Sergey ^b; Stevenson, Keith ^a; Petrov, Vladimir ^c; Troshin, Pavel ^{a,b}.
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Complex lead halides with perovskite crystal structure continue being one of the hot topics in material science. One of the main application areas for perovskite semiconductor materials are various optoelectronic devices, including solar cells and electromagnetic waves detectors. Along with simple and cheap fabrication process, complex lead halides were found to be extremely tolerant to high-energy particles (>1 MeV) as opposed to conventional inorganic semiconductor materials. While proton and electron irradiation of perovskite thin films and solar cells was thoroughly investigated, the impact of gamma rays, the most hazardous type of irradiation, is yet to be well understood.

In this talk, we will discuss radiation hardness of various types of perovskite absorber materials, which were subjected to accumulated gamma ray doses up to 1 Mrad. Mixed halide triple cation perovskite (Cs_{0.15}MA_{0.10}FA_{0.75}Pb(Br_{0.17}I_{0.83})₃) was found to undergo

substantial phase segregation similar to what was revealed for mixed halide perovskites under visible light. Solar cells based on single-halide systems such as MAPbI₃ (MA = methylammonium), MAPbBr₃, Cs_{0.15}FA_{0.85}PbI₃ (FA = formamidinium), Cs_{0.1}MA_{0.15}FA_{0.75}PbI₃, CsPbI₃, and CsPbBr₃ were found to be more resistant to high radiation doses. A particularly exciting finding was that MAPbI₃ solar cells can withstand a 1 Mrad gamma ray dose without any noticeable degradation of the photovoltaic properties. Such unusually high radiation hardness was explained by excellent material self-healing properties and supported by ab initio calculations. Given the fact that thermally unstable MAPbI₃ outperforms rigid all-inorganic perovskites in terms of stability with respect to gamma rays, it might find valuable applications in space PV technologies and gamma ray detectors.

ID: 015 Universal measurement protocol for perovskite based photovoltaic devices

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In the literature, several protocols for different PSC technologies have already been published. However, due to the vastness and variety of materials in this class they are probably not applicable to all PSC devices and technologies due to two main reasons: 1) overlapping/superimposition of light soaking and degradation effects; 2) transient effect disturbing the device equilibrium.

A new protocol to measure perovskite photovoltaic devices (PSC) was developed and here presented. This protocol does not require prior information about the device and is universally applicable. It is particularly suitable to measure record devices as often there is no prior information on their behavior. The potential degradation under illumination is minimized, by measuring the most important parameter namely maximum power first and only afterwards determine the other I-V curve parameters.

The protocol proposed in this study consists of the following steps:

- 1) Perform initial quick automatic I-V scan in forward (from I_{sc} to V_{oc}) and reverse (from V_{oc} to I_{sc}) sweep direction. Typical sweep time 15 s with 100 data points.
- 2) Stabilize the device under light at fixed voltage near V_{mp}: monitor output power (which typically improves with time with typical time scales of several minutes)
- 3) Decrease the voltage stepwise until short-circuit conditions, that is 0 V (or slightly negative, but no more than 0.2 % of V_{oc}).
- 4) Return to V_{mp} and check that output power of step 2 is reached
- 5) Increase the voltage stepwise until open-circuit conditions, that is V_{oc} (or slightly higher, but reverse current should not exceed 2 % of I_{sc}). At each step observe the output power and wait for its stabilization over time (typically within 0.2 %).
- 6) Return to V_{mp} and check that output power of step 2 and step 4 is reached

A number of devices was tested with the protocol above and results will be presented. Different PSC devices showed different behaviors. A discussion on the critical steps and how to act in the various occasions will be given.

This protocol will lead to reliable determination of PSC device performance, which also is representative of their real world performance in a PV installation. The latter might not be achieved by more traditional I-V curves determined from voltage sweeps, where the device is inherently never under steady-state conditions.

ID: 018 In Situ Investigation and Photovoltaic Devices: Sequential Formation of Tunable-Bandgap Mixed-Halide Lead-based Perovskites

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Inorganic–organic hybrid perovskite films of $\text{MAPb}(\text{I}_x\text{Br}_{1-x})_3$ ($0 < x < 1$) represents a path for efficient multi-junction or tandem solar cells due to their tunable bandgap (1.60–2.24 eV). Here, sequential solution deposition is adapted to enable a direct observation and a full understanding of the phase transformation from $\text{Pb}(\text{I}_x\text{Br}_{1-x})_2$ precursors to perovskites. This method has been successfully applied toward the fabrication of homogenous perovskite layers allowing an improvement of optoelectronic properties and device performance. In situ grazing incidence wide-angle X-ray scattering (GIWAXS) measurements are performed to present a detailed view of the effects of solvent, lead halide film solvation, and Br incorporation and alloying on the transformation behavior. Supported by other techniques such as in situ optical reflectance, absorption, x-ray diffraction, and steady-state/time-resolved photoluminescence, the measurements indicate a strong tendency of lead halide solvation prior to crystallization during solution-casting $\text{Pb}(\text{I}_x\text{Br}_{1-x})_2$ precursor from a dimethyl sulfoxide (DMSO) solvent with the Br alloying leading to weakened solvation of $\text{Pb}(\text{I}_x\text{Br}_{1-x})_2 \times \text{DMSO}$. We demonstrate a room temperature conversion of perovskite and high-quality films with tunable bandgap reaching a higher power conversion efficiency of 16.42% based on $\text{MAPb}(\text{I}_{0.9}\text{Br}_{0.1})_3$ due to highly efficient intramolecular exchange between DMSO molecules and organic cations. These findings highlight the benefits that solvation of the precursor phases, together with bromide incorporation can have on the microstructure, morphology and optoelectronic

properties of these films, providing a viable alternative approach to one-step synthesis approach used for mixed ion perovskite thin films.

ID: 020 What is killing organic photovoltaics: light-induced crosslinking as a general degradation pathway of organic conjugated molecules

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Organic solar cells nowadays is a very promising technology because it has a number of advantages such as mechanical flexibility, lightweight and unprecedented production scalability, which are hard to achieve for conventional solar panels based on silicon and other inorganic semiconductors. The photoactive layer of the most efficient solution-processible organic solar cells is usually based on the blends of a conjugated polymer and fullerene derivatives or non- fullerene acceptors. However, the photoactive layer undergoes photochemical and/or thermal degradation under the operating conditions of the solar cell. The nature and mechanisms of these degradation processes remain poorly understood. A number of reports considered the photodimerization of fullerene-based materials as the main cause of the so-called burn-in degradation of organic solar cells.

In this work, we demonstrate that different types of conjugated polymers and small molecules undergo similar light-induced crosslinking regardless of their chemical composition and structure. The experiments were carried out in a special facility for accelerated tests with UV lamps or metal halide lamps as a light source. The formation of thin films of conjugated polymers and the investigation of their photochemical degradation were carried out in an inert atmosphere inside a glove box.

It was found that photodegradation leads to the crosslinking of macromolecules and results in the formation of insoluble products. In some cases, fragmentation of polymer chains and accumulation of low-molecular compounds were also observed. The gel permeation chromatography analysis was shown to be a very simple and sensitive technique for monitoring the photochemical degradation of conjugated polymers and small molecules.

Thus, we established a very general degradation pathway leading to the crosslinking of conjugated polymers and small molecules under light exposure in the absence of oxygen and moisture, which is at least partly responsible for the undesired burn-in effect in organic solar cells. Our results shift the paradigm of research in the field toward designing a new generation of organic absorbers with enhanced intrinsic photochemical stability in order to reach practically useful operation lifetimes required for successful commercialization of organic photovoltaics.

ID: 022 Comparison of non-fullerene acceptors: How geometry influences electronic transport

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We compare several crystalline non-fullerene acceptors (NFA) for high-efficiency organic solar cells. The goal is to establish a relation between intramolecular structure and intermolecular packing, and electron mobility ¹. The molecules have acceptor-donor-acceptor (ADA) structure allowing for an efficient transport in a wire mesh topology of intermolecular packing when acceptor units are aligned in π -stacks. In the ideal packing the electronic connectivity is three-dimensional (Y6, o-IDTBR). However in known NFA some contacts are broken for different reasons resulting in a reduced dimensionality of electron transport network (EH-IDTBR, ITIC-1Cl, ITIC-2ClH). Also for some NFA we observe different polymorphs at ambient conditions having qualitatively different intermolecular packing (ITIC-Th). Interestingly, among the considered NFA, the material showing the highest calculated electron mobility in a single crystal (Y6) shows also the best solar cell performance.

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POSTERS

ID: 013 Electrochemical Impedance Spectroscopy Analysis of Lead Halide Perovskite Solar cells

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ID: 014 Advanced Characterization of Halide Perovskites using the Moving Grating Technique

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ID: 017 Simple Interfacial Passivation for HTL-free Perovskite Solar Cells with Carbon Top Electrodes

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ID: 023 Film Deposition Techniques Impact Defect Density and Photostability of MAPbI₃ Perovskite Films

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ID: 026 Influence of Backbone Fluorination on Optoelectronic and Photovoltaic Properties of Novel (X-DADAD)_n Conjugated Polymers

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ID: 027 Effect of Partial Pb₂₊ Substitution with Ca₂₊ on the Stability and Photovoltaic Performance of All-inorganic CsPbI₃ Perovskite

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ID: 028 Design of Novel Thiazolothiazole-based Conjugated Polymers for Organic Solar Cells

Proshin, Pavel * ^{a, b}; Nikitenko, Sergey ^b; Troshin, Pavel ^{a, b}; Akkuratov, Alexander ^b

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ID: 029 Liquid Metal Melt Electrodes for Low-cost Perovskite Solar Cells

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ID: 038 Improving the Operation Stability of Organic Solar Cells by Using Naphthalene Dithiol.

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ID: 039 Photochemical and Mechanical Stabilization of Organic Solar Cells Using Naturally-occurring Antioxidants

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ID: 040 The Role of the Passivation Additives in Enhancing the Intrinsic Photochemical Stability of Lead Halide Perovskites

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ID: 041 Additive Approach to Enhance Intrinsic Photochemical and Thermal Stability of MAPbI₃ Thin Films

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ID: 042 Polymer-based organic photovoltaic modules for powering wireless smoke sensors under indoor illumination conditions

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ID: 043 A-site Cation Engineering in Two-dimensional Ruddlesden-Popper Perovskite Films

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ID: 044 Conjugated Polymers for Stable and Efficient Perovskite Solar Cells: in Search of the Perfect Match

Tepliakova, Marina *^{a, b}; Akkuratov, Alexander^b; Klimovich, Irina^{a, b}; Kuznetsov, Ilya^b, Troshin, Pavel^{a, b}

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ID: 045 Alternating Thiophene-Benzothiadiazole Oligomer as Electron Transport Material for Inverted Perovskite Solar Cells

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ID: 046 Study of the Hydrophobicity Effects within Quasi-solid-state Hybrid Photovoltaic Devices

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ID: 047 Partial Substitution of Pb₂₊ with Other Metal Cations as an Efficient Strategy to Improve the Photostability of CsPbI₃ Perovskite Films

Ustinova, Marina *^{a, b}; Mikheeva, Maria^{c, a}; Shilov, Gennady^b; Dremova, Nadezhda^b; Frolova, Lyubov^{a, b}; Aldoshin, Sergey^b; Stevenson, Keith^a; Troshin, Pavel^{a, b}

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ID: 048 Lead or Organics: a Comparative Toxicity Assessment for Precursor

Materials used in Perovskite Solar Cells

Chetyrkina, Margarita*^{a, b}; Kameneva, Larisa^b; Klimanova, Elena^c; Sashenkova, Tatyana ^c; Allayarova, Ugulzhan ^c; Mishchenko, Denis ^c; Kostyuk, Svetlana ^b; Troshin, Pavel ^{*a, c}

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ID: 049 Improving Stability of Perovskite Solar Cells Using Conjugated Polymer-fullerene Derivative Composite as Electron Transport Layer

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ID: 050 Design and Investigation of Triarylamine Derivatives as Hole Transport Materials for Perovskite Solar Cells

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ID: 051 Embedded Current Collectors for Efficient Large Area Perovskite Solar Cells

Duarte, Vera ^a; Ivanou, Dzmitry ^a; Bernardo, Gabriel ^a; Andrade, Luísa; Mendes, Adélio*^a

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ID: 052 Scalable Slot-die Coating for Perovskite Solar Cells Deposited under Ambient Conditions

Carvalho, Tânia ^a; Andrade, Luísa ^a; Mendes, Adélio *^a

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ID: 053 Non-linear Band Gap Dependence of Mixed Pb-Sn 2D Ruddlesden-Popper Perovskites

Underwood, Cameron^a; Carey, J. David ^a; Silva, S. Ravi P.*^a

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ID: 054 Novel Star-shaped Donor-acceptor Molecules Based on Triphenylamine for Organic Solar Cells and Photodetectors

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ID: 055 Design of PV-grade Functional Materials for Perovskite Solar Cells

Mumyatov, Alexander *^{a,b}; Akkuratov, Alexander ^{a,b}; Kuznetsov, Ilya ^{a,b}; Tsarev, Sergey^c; Elnaggar, Mohamed ^c; Prudnov, Fedor ^{c, a, b}; Frolova, Lyubov ^{c, a, b}

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ID: 056 The Electrochemical Stability of P-I-N Perovskite Solar Cells Assembled Using Different Electron-transport Layer Materials

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ID: 057 Novel Donor Small Molecules Based on Benzotriindole: Synthesis, Properties and Application in Organic Solar Cells

Balakirev, Dmitry O.*^a; Luponosov, Yuriy N.^a; Mannanov, Artur L.^a; Savchenko, Petr S.^a; Peregudova, Svetlana M. ^b; Paraschuk, Dmitry Yu ^{a, c}; Ponomarenko, Sergei A. ^a

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ID: 058 Unveiling the Electronic State Interplay at the DBP/4P-NPD Interface in Organic Solar Cells

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ID: 059 Efficiency Enhanced Industrial-Compatible Organic Photovoltaics using Roll-To-Plate (R2P) Nanoimprint Lithography

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ID: 060 Novel Benzodithiophene-based Push-pull Copolymers for Organic Solar Cells

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ID: 061 Novel Impedance Photocurrent Microscopy Setup for Next Gen Photovoltaics

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