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HEAVY-METAL FREE SEMICONDUCTOR NANOCRYSTALS FOR PHOTOCATALYTIC APPLICATIONS

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ABSTRACT

Semiconductor nanocrystals (NCs) are emerging as promising photocatalysts owing to their large surface-to-volume ratios and tunable physicochemical properties. These attributes position them as attractive candidates for solar-to-fuel conversion and for use across environmental, chemical, and biomedical photocatalytic technologies. Although earlier research has largely focused on Cd-based semiconductor NCs, concerns related to toxicity, environmental impact, and regulatory limitations restrict their widespread adoption. To address these challenges, this lecture will present several strategies for advancing photocatalysis using heavy-metal-free semiconductor nanocrystal systems, with particular emphasis on photocatalytic water splitting for green solar fuel production.

First, we introduce large wurtzite InP nanocrystals synthesized via cation exchange and demonstrate their use in a "tandem-like" configuration that enables efficient harvesting of the red portion of the solar spectrum. Second, we discuss the role of metal co-catalysts grown on NC surfaces and examine how their structural and electronic interactions influence photocatalytic performance, with special attention to the single-atom catalyst regime. Third, we explore hybrid systems that integrate semiconductor nanocrystals with polymeric carbon nitride photoelectrodes, forming NC-meets-CN architectures that exhibit synergistic enhancements in photoelectrocatalytic function.

Together, these approaches highlight new pathways toward efficient, sustainable, and heavy-metal-free photocatalytic nanocrystal systems.

Electronic Origins of Charge-Carrier Yields in Transition-Metal Oxide Photoabsorbers for Solar Fuel Generation

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Transition metal–oxide semiconductors are promising photoabsorbers for solar-fuel generation. Although champion photoelectrodes based on oxides with d^0 and d^{10} electronic configurations exhibit high internal quantum efficiencies, their band gaps are typically too large for practical applications. In contrast, metal-oxides with open d-shell configuration often have solar-relevant band gaps but suffer from significantly lower photoconversion efficiencies. To understand the origins of these losses, we combine epitaxial thin-film growth, optical spectroscopy, photoelectrochemistry, and time-resolved microwave conductivity (TRMC), to shown that open d-shell oxides suffer from intrinsically limited mobile charge-carrier yields, with a substantial fraction of absorbed photons failing to generate carriers capable of driving redox chemistry. Comparative measurements on photoanodes composed of epitaxial thin film Fe_2O_3 polymorphs, α-Fe_2O_3 (hematite) and β-Fe_2O_3, demonstrate that, although crystal structure strongly affects carrier transport, the carrier yields and their spectral profiles remain essentially unchanged, indicating that the dominant loss mechanisms likely arise from intrinsic ligand-field (LF) states rather than differences in long-range crystalline structure. Consistent with this picture, we find that Ti doping modestly improves carrier yields in hematite, although the overall limitations imposed by LF states remain. Extending this approach to complex Fe-based oxides such as $ZnFe_2O_4$ reveals similar carrier yields, confirming that non-unity mobile carrier generation is a general feature of Fe-based oxides and not specific to Fe_2O_3. To further probe the electronic origins of these losses, we examine a broader class of ilmenite-type $MTiO_3$ oxides (M = Ni, Co, Mn), where the transition-metal d-electron configuration systematically tunes the balance between LF and ligand to metal charge-transfer (LMCT) transitions. Across this series, mobile charge carriers arise primarily from $O^{2-} \rightarrow Ti^{4+}$ LMCT transitions, whereas LF excitations introduce relaxation pathways that do not generate mobile carriers. These results indicate that the balance between LF and CT excitations plays an important role in determining carrier yields in open d-shell metal-oxides, providing useful direction for efforts to improve solar-fuel devices based on transition-metal oxides

Optoelectronic Characterization of Molecule-Terminated Photoelectrodes

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Abstract:

Molecular monolayer termination of semiconductor surfaces offers a powerful and versatile route for engineering interfacial charge transport by directly tailoring surface electronic structure. Through the introduction of surface dipoles and the chemical passivation of dangling bonds, molecular functionalization enables precise control over band-edge energetics, defect states, and charge-transfer barriers, thereby enhancing the performance of a broad range of electronic and optoelectronic systems, including photo(electro)chemical cells (PCE). In PEC architectures, where charge transport is dictated by band-edge alignment with electrolyte redox potentials, silicon emerges as a particularly compelling photoelectrode material. Its optimal 1.12 eV band gap enables broadband solar absorption from the UV to the near-infrared, allowing Si to harvest a significantly larger fraction of solar photons than wide-band-gap semiconductors such as TiO_2 and GaN. Importantly, the ability to form well-passivated hydrogen-terminated Si surfaces provides an ideal platform for robust molecular modification, offering an additional and tunable degree of freedom for controlling interfacial energetics and charge-transfer dynamics.

By integrating experimental spectroscopy, electrochemical measurements, and theoretical modeling, the work reveals that molecular dipoles induce well-defined shifts in band-edge energetics in air, while exhibiting reversed trends at semiconductor/electrolyte interfaces due to Fermi-level alignment and interface states. Hydrogen-terminated Si is shown to generate a consistent surface dipole independent of doping, whereas molecular passivation layers introduce a synergistic interplay between electronic band bending and chemical transport barriers that critically determines metal catalyst electrodeposition kinetics. Collectively, these findings establish surface chemical modification as a powerful design principle for engineering interfacial energetics, minimizing recombination losses, and maximizing charge-transfer efficiency in silicon photoelectrodes, advancing the rational design of high-performance organic–inorganic hybrid interfaces for solar-driven energy conversion.

Reshaping Synthesis Strategies for Metal Oxide Semiconductors: From Binary to High-Entropy Systems for Solar Fuel Applications

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The advancement of photocatalytic systems for solar fuel production requires careful control over the structures and properties of metal oxide semiconductor materials. In this talk, I will present integrated synthesis strategies that combine Physical Vapor Deposition with Rapid Photonic Annealing, demonstrating how these methods address different material challenges across the semiconductor synthesis spectrum to unlock the potential of solar fuels.

Using Bi_2O_3 as a model binary system (chosen for its relatively accessible processing temperatures and well-characterized polymorphism), we demonstrate kinetic control of crystal polymorphism through Flash Photonic Heating (FPH, heating rates of 10^6-10^7 °C/s), achieving reversible α↔β phase transformations. Polymorphism control is crucial because metastable phases often have superior optoelectronic properties. β-Bi_2O_3 has enhanced photocurrent density and reduced bandgap compared to the thermodynamically stable α- Bi_2O_3. Pulsed laser deposition improves film quality by delivering much higher energies than chemical methods for precise stoichiometric control, while FPH enables polymorph control at accessible temperatures, providing insights into kinetic versus thermodynamic crystal-formation pathways.

At the opposite end of the synthesis-complexity spectrum, high-entropy rare earth oxides (HEREOs) such as $(Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Y_{0.2})O_2$ require integrated strategies to fulfill their potential for enhanced catalytic performance and structural stability. These chemically complex, refractory materials require the combined high-energy deposition techniques of physical vapor deposition and the unique thermal processing capabilities of rapid photonic annealing to ensure high crystallinity and controlled nanostructuring. FPH enabled forming nanoscale grains and increased surface area, unlocking the catalytic potential crucial for next-generation energy conversion systems.

This materials-spanning approach shows how synthesis requirements shift from controlling polymorphs for better optoelectronic properties in binary systems to integrated nanostructuring strategies for improved catalytic performance in high-entropy materials. The presentation will illustrate how understanding these different challenges offers key pathways for developing advanced metal oxide semiconductors for solar fuel applications.

Advances and Challenges in Rechargeable Aqueous-Based Batteries

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Abstract

With the accelerating deployment of renewable energy technologies, the demand for efficient, safe, and environmentally compatible energy storage solutions continues to grow. This has driven increasing interest in developing new rechargeable battery systems that combine low cost, high safety, long-term stability, and the use of earth-abundant materials. Among these aqueous-based batteries have emerged as a promising alternative for developing safe and sustainable rechargeable batteries. Their water-based electrolytes provide intrinsic nonflammability and material sustainability, while supporting a wide range of electrode chemistries. However, these systems still face challenges that include corrosion, hydrogen evolution and other side reactions that reduce efficiency and cycle life. In this talk I will discuss recent advances in understanding and improving aqueous batteries across multiple material classes. I will highlight our work on controlling ion solvation, electrolyte composition and interphase formation in order to improve the stability and reversibility of anode systems. We show how changes in the local solvation environment guide the structure of the interphase and regulate water activity. These factors have a significant influence cell performance including self-discharge, charge efficiency and cycle stability. These insights help to improve our understanding of how aqueous batteries operate and point to design principles that can support progress in their stability and performance.

Design and Application of Aerogel-based Catalysts for the Oxygen Reduction Reaction in Fuel Cells

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Among the key physical and chemical properties required from catalysts and catalysts' supports for fuel cell and water electrolyzers are high surface area and electronic conductivity. These have been limiting factors in the design of advanced materials for energy production and storage. In the past decade I have been focusing my research on designing advanced 3D materials' frameworks based on aerogels.
During these years, I developed three main categories of aerogel-based materials for fuel cells and water electrolyzers: inorganic covalent frameworks, metal oxides, and ceramics. These have been used for catalyzing the oxygen reduction reaction in fuel cells, the oxygen evolution and hydrogen evolution reactions in water electrolyzers and hydrogen pumps, and as corrosion-resistant catalysts' supports in fuel cells. In this talk I will share our journey in the development of inorganic covalent aerogels, from the design criteria, synthesis and application of some of the state of the art catalysts for oxygen reduction in fuel cells.

Photocatalytic panels development for catalytic oxidation and reduc-tion reactions

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Heterogeneous photocatalysis is an attractive enabler of the efficient execution of various im-portant environmental (e.g., hydrogen production and C-based fuel production) and organic reac-tions utilizing solar energy. In a typical batch reactor, a heterogeneous photocatalyst is dispersed in a given solution together with reactants, and upon illumination, a chemical reaction occurs. Despite its simplicity, the overall process faces some challenges related to the intrinsic nature of the reaction conditions: light penetration significantly decreases with distance, the photocatalyst should be continuously stirred to avoid sedimentation, separating the products from the photocata-lyst is not trivial, the catalyst is hard to recycle, the reaction is dependent on the concentration of starting reactants, and scalability is questionable.

An alternative approach is to use a panel based on a photocatalytic material. This configuration enhances light management and facilitates easy recycling and scalability, similar to that of solar cells. Furthermore, the photocatalyst panel can be easily incorporated into a continuous-flow re-actor, facilitating constant reactant feed and product separation. In recent years, polymeric carbon nitride (CN) materials have emerged as a class of photocatalysts for many reactions, from solar fuel production to biomass conversion and complex organic transformations. Nevertheless, most studies have focused on using CN powders as heterogeneous photocatalysts. Some pioneering works have shown the utilization of CN panels, primarily for H_2 production. However, all these panels were prepared by drop-casting or screen-printing a synthesized catalyst with a polymer containing perfluoro groups (i.e., Nafion) or a SiO_2 binder onto frosted glass or steel plates. The use of a binder can lead to photocatalyst detaching from the substrate due to the formation of radicals during the reaction, such as reactive organic species (ROS). This phenomenon primarily occurs in organic chemical reactions, where ROS intermediates can react with the binder to pro-duce unwanted byproducts.

This talk will introduce facile and scalable approaches for growing polymeric carbon nitride (CN) layers on conductive substrates with tunable structural and photophysical properties for photocata-lytic applications. We demonstrate CN-based photocatalytic panels as highly stable, efficient plat-forms for converting organic molecules into value-added chemicals while simultaneously produc-ing hydrogen and hydrogen peroxide. Additionally, I will demonstrate the use of CN-films as highly stable photocatalytic panels for various catalytic and cascade reactions.

The Effect of Row Spacing and Albedo on the Power Production of a Bifacial Solar Panel Array

Avi Niv, Sophie Binman and Amnon Schur
Dead-Sea Works, Sedom, Israel

Abstract

The rapidly increasing adoption of bifacial photovoltaic (PV) technology highlights a critical gap in knowledge regarding optimal array configuration and performance prediction. Unlike monofacial modules, the energy yield of a bifacial solar panel array is **highly sensitive to inter-row shading**, which is governed by the array's row spacing and ground clearance. This sensitivity creates a challenging trade-off: dense packing maximizes the number of production units per land area, while wider spacing minimizes shading, thereby increasing individual panel productivity. To determine the conditions for **maximum overall array power production**, this study employs a combined simulation and experimental approach focusing on row spacing and ground albedo.

Initial analysis using the **Bifacial-Radiance** ray tracing tool modeled a three-row array [1]. Simulation results demonstrated that increasing row spacing from 2 to 6 meters yields a moderate change in front-side annual radiance, but a dramatic increase in rear-side radiance, confirming the non-linear dominance of inter-row shading on the bifacial gain.

To empirically validate and extend these findings, two parallel **three-row test fields** have been constructed in Sedom region in Israel – A region known for its exceptional solar irradiance and unique desert conditions. Both fields allow for **variable row spacing (3.5 to 6 meters).** Crucially, the fields are differentiated by their ground conditions: one is built over native ground and the second is laid over a thick layer of high albedo clear salt to isolate the impact of ground reflectivity.

At the conference, we will review the initial operational data collected from **November 2025 through February 2026**. This data will detail power production performance under different row spacing and albedo conditions, analyzing variations between central and side panels in each row. The study's culmination will be the **derivation of empirically grounded design guidelines** intended to aid in the high-yield deployment and optimization of utility-scale bifacial PV projects.

Keywords: Bifacial PV, Row Spacing, Array Optimization, Albedo, Shading Loss, Bifacial-Radiance.

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Mapping the Spatial Contribution to Photoluminescence and Photovoltage in Perovskite Solar Cells

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Lead halide perovskites have emerged as promising candidates to replace silicon in photovoltaic technologies, owing to their tunable direct bandgap, strong absorption, and low-cost fabrication. Despite their high photocurrent, further improvement in open-circuit voltage is required to approach efficiency limits. This calls for advanced operando characterization techniques capable of mapping the specific contributions to device photovoltage.

Here, we combine photoluminescence quantum yield (PLQY) measurements with optical modeling to investigate charge separation and recombination processes in perovskite solar cells. We introduce the spatial external luminescence efficiency (SELE), the probability that a photon generated at a given depth escapes as measurable photoluminescence, as a powerful tool to gain insights into local loss mechanisms[1].

By comparing SELE profiles across devices, we map factors influencing PLQY and show that variations at the PEDOT:PSS/perovskite interface strongly affect performance. These interfacial variations, originating from fabrication processes, align with reported photovoltage fluctuations in solution-based cells[2] and arise from trap states[3], surface band bending, and mismatched quasi-Fermi level splitting[4].

Our spatial mapping approach reveals how interfacial quality governs charge separation and recombination dynamics, where improved interfaces enhance luminescence and photovoltage, while poor ones limit carrier diffusion and suppress external emission. This methodology enables spatial quantification of radiative versus non-radiative recombination, distinguishing bulk from surface-driven losses, and provides valuable insight for advancing perovskite solar cell performance.

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Liberating Molecular Excitons by Confined Photons

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The poor transport properties of organic semiconductors are often considered as the Achilles' heel of these materials, placing severe limitations on the performances of organic-electronics devices. However, by embedding them in resonant photonic structures, their wavefunctions can be hybridized with light to create composite quantum excitations, which are partly photonic and partly excitonic.

In this talk I will show how this entanglement between light and matter can provide a novel pathway for enhancing the transport properties of materials, boosting the typical transport range from several nanometers to tens of microns. Furthermore, I will present our ultrafast time-resolved imaging measurements, where we revealed that the hybrid light-matter excitations exhibit a mobility transition between different types of transport mechanisms, governed by their composition. These results provide crucial insight into the mesoscopic quantities governing cavity-enhanced transport and pave the way towards novel organic electro-optic devices harnessing the coherent interaction between light and matter.

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Towards Sustainable Practices in Photovoltaic and Agricultural Greenhouse Systems: An Ecosystem Services Framework

Steren, A., Slater, Y., Rubin, O. D., Fleischer, A., & Kan, I.

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Abstract

Policies promoting agrivoltaics face the challenge of balancing between mitigating climate change and farmland preservation. This study applies an ecosystem-services (ESS) approach to evaluate the introduction of transparent solar panels (TSP) as photovoltaic and agricultural greenhouse systems (PVGs) with low impact on agricultural activities. Using a partial equilibrium model of Israel's vegetative agriculture, we simulate the introduction of TSP on farmers' optimal land allocation between open-field and covered crops and its sustainability. The model accounts for food and energy production as provisioning vegetative-agriculture ESS (VAESS), and for greenhouse-gas (GHG) emissions and open-field landscape as non-provisioning VAESS. Our findings suggest that TSP represents an economically viable and sustainable PVG technology. The adoption of TSP, alongside policies that internalize the value of non-provisioning ESS, is projected to convert 1.3% of Israel's cultivable land from open fields to covered crops, contributing approximately 7% to the nation's electricity supply. The estimated annual increase in VAESS per hectare is valued at $864, comprising $812 from electricity generation, $259 from GHG emission reductions, $277 in consumer surplus from agricultural products, offset by a $441 reduction in agricultural output, and a $43 decrease in landscape value. Our analysis demonstrates how an ecosystem services framework can guide policy decisions toward optimal land-use allocation in agrivoltaic systems.

Solar to hydrogen generation using thermoelectric energy conversion

Yaniv Gelbstein, The Dean of the Faculty of Engineering Sciences, BGU

Abstract

An effective conversion of solar energy into 'green' electricity can drive a solid oxide electrolyzer cell, splitting water into oxygen and hydrogen. The generated hydrogen can be stored in solid state MgH_2, while being released on demand and converted back to electricity by a solid oxide fuel cell. The current research activity involves state-of-the-art thermoelectric materials and devices for enhancing the photovoltaics' and solid oxide cells' efficiency and an electronic control system, optimizing the power output of each component.

The talk will be focused on the entire supply chain from solar to hydrogen, with a detailed focus on the role of thermoelectric materials in optimizing efficiency via hybrid photovoltaic-thermoelectric and solid oxide cells-thermoelectric devices. Recent achievements in development of advanced thermoelectric materials will be described.

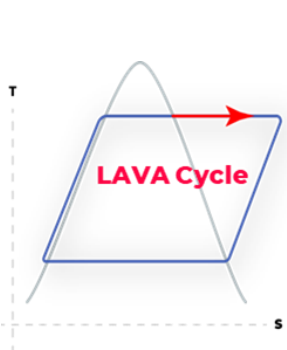
Why Isothermal Heat Engines and Heat Pumps Are the Future of Photovoltaics, and Batteries

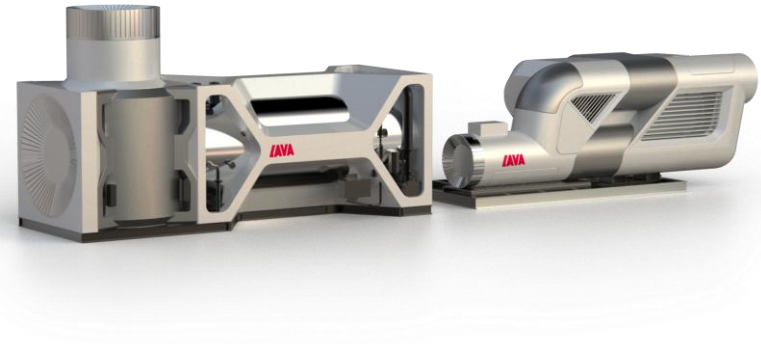
Prof. Carmel Rotschild, Mechanical Engineering, Technion & CTO, LAVA Power

Abstract

Carnot-efficient engines have the theoretical potential to double electricity production efficiency. However, achieving true isothermal expansion in conventional systems—where gases with inherently low heat capacity are used—typically results in negligible power output. We have developed a novel isothermal heat engine that overcomes this limitation by utilizing bubble expansion within a heat transfer liquid, enabling near-perfect isothermal heat exchange. The resulting gas–liquid mixture is accelerated through a converging–diverging nozzle, converting thermal energy into kinetic energy to drive a reaction turbine and generate electricity.

Building on this principle, we have also designed an isothermal compression heat pump based on similar physics. Together, these disruptive technologies offer transformative solutions for waste heat recovery, geothermal energy, small modular reactors (SMRs), heating, and cooling. They also form the foundation of the Carnot battery—a system capable of converting any renewable energy source into a fully dispatchable, standalone power supply.





How can solar energy emerge from its own success trap

Gideon Friedmann, NetZero Tech Ventures

Solar energy has by far the highest renewable energy (RE) installed capacity today (>2,000GW, vs 1,300GW of hydropower and 1,150 of wind power) compared to a negligible number just 20 years ago. However, except for the introduction of bifacial panels, the PV technology has not changed from its inception.

The reason for this success is the cost. From LCOE of $0.45 to $0.04 (world average) over the last 20 years, with installation costs going down from $6,000/KW to $800/KW. This is coupled with the development of large-scale storage, and a similar cost reduction there (still going on).

It is interesting to compare the advent of solar and storage. They both share similarity of scalability. The basic module is very small, and large units just comprise of an enormous amount of the small module – thousands to millions. In both cases the cost reduction comes mainly from economies of scale achieved by very well-engineered industrial manufacturing. Unfortunately, this also meant that China, which excels in this, is the dominant player in both industries.

(a brief description of current PV technologies (other than silicone) – CIGS, OPV, CdTe)

So, is it all well? Certainly, the situation is quite all right – the world can continue to rely on PV to provide the lowest cost electricity. But can we do better? If we analyze the system installation costs, we see that the PV modules cost between 20-25% of the system installation costs in utility scale installations (much less in smaller systems). This leads to the immediate conclusion that we need not direct our research to reducing the module costs, because it will have a marginal effect on the cost of PV electricity. The only technology improvement that will have a significant impact is increasing the PV module efficiency – because it relates linearly to the electricity cost.

The very well-honed industrial manufacturing process – and the excellent long-term performance of silicone PV, is a deterrent to new investors. Because any new technology needs to reach at least the same LCOE, and with the giant players continuously investing in improving their technology, any hope for new technology will clearly need a long time to industrialize + compete with the then current technology. Investors are very hesitant to take a risk on such technologies.

So, is it all lost? I don't think so – but it is certainly challenging. Research should focus on efficiency, but from physics, it seems that we are not very far from the practical maximum single material conversion efficiency. So, we must take a multi-layered approach. 2 current directions seem interesting: Tandem cells, and quantum dots. Another important direction is agri-voltaics, some way of splitting the energy efficiently is a good direction for innovation.

Detecting and Typifing PV Adoption Dynamics Using Deep Learning SPYSAM Pipeline

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Understanding how PV adoption unfolds over time is essential for designing targeted interventions and tailored strategies that accelerate energy transitions, particularly in marginalized off-grid regions where energy poverty remains acute. Yet, in many such communities there is no systematic documentation of the extent, timing, and spatial distribution of PV deployment, which severely limits the ability to explore their unique adoption processes. Recent advances in deep learning offer a path to overcome this challenge, as automatic computer vision methods can now extract precise and comprehensive information by utilizing remote sensing imagery.

Here, we developed SPYSAM, a target-specific pipeline that fine-tunes integrated pretrained state-of-the-art foundation models - YOLOv9 for object detection and SAM for segmentation - to generate spatio-temporal detection of small-scale PV systems across the informal off-grid Bedouin settlements in the Negev, by using 0.14-0.24 m resolution aerial photos. SPYSAM achieves high segmentation accuracy, with F1 scores ranging from 0.82 to 0.91 and balanced precision-recall performances.

The data harvested by SPYSAM pipeline enabled the development of a time-series analytical framework for quantifying and typifying PV adoption dynamics. At the core of this framework is ATI, a newly developed metric that captures cumulative adoption intensity over time for each entity. ATI, combined with three additional key adoption features, enables construction of an eight-adoption-dynamic typology that identifies stagnating and declining paths, leaping trajectories, lagging behavior and two distinct front-runner paths. Identification of these diverse behaviors carry direct policy implications, enabling the design of context-specific fostering-measures for communities that require active support to initiate adoption, for settlements that fail to realize their full adoption potential, or for those experiencing stalled or deteriorate phases, and facilitating detection of localized imitation hubs that may serve as influential cores.

Beyond adoption dynamics typology, ATI serves as a robust foundation for systematic and quantitative models for analyzing barriers and facilitators that shape adoption processes, including spatial, infrastructural, socio-economic, and geopolitical drivers. This examination provides deeper insight into the mechanisms that govern energy transition, particularly in marginal regions.

Ratchet based Ion Pumps for selective ion separations

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Even though highly selective ion pumps are found in the membrane of every living cell, artificial ion selective separation is a longstanding unmet challenge in science and engineering. The development of a membrane-based ion separation technology can drive dramatic progress in a wide range of applications such as water treatment, bio-medical devices, extraction of precious metals from sea water, chemical sensors, solar fuels and more. In this contribution we report the experimental demonstration of ion pumps based on an electronic flashing ratchet mechanism.

Electronic flashing ratchets are devices that utilize a temporal modulation of a spatially asymmetric electric field to drive steady state current. Like peristaltic pumps, where the pump mechanism is not in direct contact with the pumped fluid, electronic ratchets induce a net current with no direct charge transport between the power source and the pumped charge carriers. Thus, electronic ratchets can be used to pump ions in steady state with no electrochemical reactions between the power source and the pumped ions resulting in an 'all-electric' ion pump.

Ratchet-based ion pumps (RBIPs) were fabricated by coating the two surfaces of nano-porous alumina wafers with gold, thus forming nano-porous capacitor-like devices. The electric field within the nano-pores is modulated by oscillating the capacitor voltage. Thus, when immersed in a solution, ions within the pores experience a modulating electric field resulting in ratchet-based ion pumping. The RBIPs performance was studied for various input signals, geometries, and solutions. RBIPs were shown to drive ionic current densities of several $\mu A/cm^2$ even when opposed by an electrostatic force. A significant ratchet action was observed with input signal amplitudes as low as 0.1V thus demonstrating that RBIPs can drive an ionic current with no associated redox reactions.

An important hallmark of ratchets is the ability to invert the direction of particle flow with a change in the input signal frequency. The stopping frequency, which is the frequency at which the particle flux changes its direction, is determined by the potential distribution and particles transport properties. As a result, for a given ratchet, there can be a frequency at which particles with the same charge, but different diffusion coefficients, are transported in opposite directions. This concept, that was never applied to ion separations, can enable the extraction of ions with extremely low relative concentrations if their diffusion coefficient is even slightly different from the main ions in the solution. We show by simulation, that for the prevalent ions in water, ions with a relative diffusion coefficient difference as small as 1% can be driven to opposite directions with a velocity difference as high as 1.2 mm/s. Since the direction of ion transport is determined by the input signal frequency, the sorting properties can be tuned in real time providing a simple fit-to-purpose solution for a variety of ion separations applications.

Sensorless Optimization of Crop-Aware Photovoltaic Tracking for Greenhouse Agrivoltaics

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Greenhouse agrivoltaics (GAPV) offers a dual-use pathway for agricultural production and solar electricity generation, yet dynamically balancing photovoltaic (PV) output with crop light needs typically relies on sensor networks, real-time feedback, and complex control systems. These requirements increase cost, maintenance, and failure risk, posing a major barrier to large-scale deployment in commercial greenhouse environments. To address this challenge, this study introduces a sensorless dynamic optimization framework that generates monthly diurnal PV tilt schedules using only climatic data, greenhouse geometry, and crop-specific Daily Light Integral (DLI) and Photosynthetic Photon Flux Density (PPFD) thresholds, eliminating the need for in-situ sensors. Radiative-transfer simulations were performed for sun-tracking, fixed-horizontal, and reverse-tracking configurations across 400 crop-level irradiance points. These simulations informed the development of surrogate irradiance models (R^2 = 0.982–0.997), enabling rapid internal-irradiance prediction without repeated ray tracing. The optimal PV tilt angle at each time interval was determined by fitting a second-order polynomial to the irradiance values of the three simulated configurations and solving for the angle that best matched the target crop irradiance for that period. Applying this framework to two hypothetical cucumber cultivation cycles showed that optimized tracking schedules maintained DLI targets of 5–15 $mol \cdot m^{-2} \cdot d^{-1}$ for seedlings and 20–30 $mol \cdot m^{-2} \cdot d^{-1}$ for growth and fruiting. Achieved DLI values ranged from 12.7 to 29.9 $mol \cdot m^{-2} \cdot d^{-1}$ in winter–spring and 16.8 to 24.8 $mol \cdot m^{-2} \cdot d^{-1}$ in late summer.

Despite prioritizing crop illumination, the optimized tracking produced 45,982 $kWh \cdot yr^{-1}$, equivalent to 97% of fixed-horizontal and 72% of full sun-tracking energy yield. By removing sensor dependence while preserving high agronomic and energy performance, this sensorless optimization framework offers a scalable, low-complexity, and robust strategy for crop-responsive PV operation in greenhouse agrivoltaic control systems.

Experimental investigation of agrivoltaic collector array with spectral beam splitting

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Agrivoltaics (APV) with spectral splitting has been studied over the past decade for its dual potential in crop production and electricity generation. This approach allows photosynthetically active radiation (PAR) to pass through the solar collectors and reach the ground. Some of these studies investigate concentrating APV systems, allowing the transmittance of different fractions of solar radiation and diffuse light to the crops. While these systems could improve overall land productivity, their practical application is still being evaluated because of the high costs associated with accurate tracking mechanisms, curved reflectors, and active cooling elements.

In the current study, the optical and electrical performance of a unique collector design is fully tested. The design includes a commercial bifacial photovoltaic (PV) panel and two planar spectrum-splitting reflectors. The technology's advantage has already been demonstrated through a detailed evaluation of the electrical and optical outputs of a large-scale field using this specific collector. The experimental set-up includes one collector row, integrated from three off-the-shelf bifacial PV panels connected in series (string) and two types of high-grade filters (hot mirror, dual band-pass), specifically designed and fabricated for the agrivoltaic application. Measurements include incident fluxes on the PV panels from both sides, panel temperature, and electrical metrics, as well as the radiation flux reaching the ground. The theoretical predictions for both the incident light and electrical output were successfully validated by the experimental data.

The empirical observations verify (1) the performance of bifacial PV panels receiving equal filtered sunlight from both sides and (2) that the current optical-thermal-electrical performance model can predict the output of a string of panels integrated in the envisioned collector. The results support the development of APV systems with better crop yield and electrical performance.

The role of the A-site cation in determining electronic properties of lead halide perovskites

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Abstract:

The A-site cation was initially considered to be a "placeholder", stabilizing the structure of lead halide perovskites. I will discuss two reflections of the importance of the A-site cation on determining electronic properties. The first has to do with exciton-exciton interactions in weakly quantum confined nanocrystals. We show that the identity of the A-site cation dramatically affects the quantum yield of the doubly excited states, and postulate that this is due to a dramatic difference in the carrier localization regime due to anharmonic lattice motion, driven by the A-site cation. The second has to do with self-healing dynamics. We show that the A site cation strongly modulates self-healing rates and dynamics, and that mixing of A-site cations affects these in unexpected ways. Together all these point at the fact that coupling of electronic and lattice degrees of freedom can lead to a dramatic role of the A-site cation, and possibly explain the observation of enhanced photovoltaic performance of cells with mixed A-site cations.

The influence of anharmonicity and magnetic doping on the electronic properties of halide perovskites

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The discussed work deals with the control and characterization of the photo-generated carriers in halide perovskite (HPs) materials via magnetic doping. The materials under consideration, $CsPbBr_3$ and PEA_2PbI_4, include the diluted concentration of Ni^{2+} or Mn^{2+} ions at a metal substitution position. Magnetic doping was implemented extensively in colloidal quantum dots, but with a limited way in the perovskite semiconductors, showing benefits in various opto-electronic and spin-related devices, including spin-LED[1], solar cells [2] and memory/information applications.

Our work reports a thorough investigation of spin degrees of freedom in the mentioned materials, monitored by magneto-photoluminescence and optically detected magnetic resonance (ODMR) spectroscopies, which provide significant information on the exact location of host carriers and dopants, as well as examine interactions between them, exposing the merits which make the magnetic HPs building blocks for the mentioned applications [3].

More specifically, one project focused on a thorough investigation of the influence of Ni^{2+} dopants on the optical and magneto-optical properties of $CsPbBr_3$ nano-cubes. The study implemented methodologies that are applied to halide perovskites for the first time, like steady-state and transient optically detected magnetic resonance (ODMR) spectroscopy, leading to significant advances that address long-standing debates in this field: (a) A direct identification of defect centers, in conflict with the widely assumed defect-free behavior of halide perovskites; (b) Direct observation of spin-exchange interactions between dopant unpaired electrons and photo-generated carriers, which has not been resolved previously. The extracted physical parameters from the ODMR experiments included: g-factors and their anisotropy, spin exchange interactions, angular momentum, carrier-dopant coupling constants, and radiative and spin-lattice relaxation times. A second project focused on the influence of Mn^{2+} dopants in 2D MA_2PbI_4 and PEA_2PbI_4 single crystals, implementing the mentioned magneto-optically spectroscopies, focusing on the added values of the dopant to the so-called Rashba effect (an ongoing project). The spin properties mentioned here undoubtedly can play an important role in the development of new functions for technologies.

[1]http://pubs.acs.org/journal/aelccp
[2]https://doi.org/10.1021/acs.jpclett.5c00005
[3]https://doi.org/10.1021/acs.chemmater.1c03822

Accurate solid-state band gaps and optical absorption spectra from density functional theory

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Abstract

Bandgaps and absorption spectra in the solid state are among the most important properties for determining the usefulness of materials in applications like photovoltaics and photocatalysis. Ideally, we would like to deduce these properties from first principles calculations. However, the workhorse of such calculations, namely density functional theory (DFT), has traditionally struggled - even qualitatively - in the description of electron and optical excitations. Specifically, the bandgap of semiconductors and insulators has been thought to be outside the reach of DFT even in principle, and the associated optical absorption spectrum outside the reach of time-dependent DFT with standard approximate functionals. Charge transfer excitations have also presented significant difficulties in both molecular and solid-state systems.

Here, a novel approach to overcoming these difficulties, involving Wannier-localization based optimal tuning of a screened range-separated hybrid functional, is presented. It is shown that quantitative accuracy for a wide range of systems, from molecules to 3d and 2d materials, is achieved without any empiricism. This opens the door to many DFT-based true predictions of electronic and optical properties, to high-throughput calculations.

Gaining control over MXene – Halide Perovskite integration chemistry for designing composite films with a target functionality

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The integration of Halide Perovskites (HaPs) with MXenes, which represents an outstanding family of highly tunable 2D materials [1], allows promoting better HaP crystallinity, passivating grain boundaries, mitigating ion migration, and tuning the work function, which enables controlling the band alignment. All these factors lead to significant advances in shelf-life and Power Conversion Efficiency (PCE) of the respective HaP-based devices [2]. However, the exact interaction chemistry of MXenes and HaPs is poorly understood, which limits the rational design of MXene-HaP composites.

In this thorough study of $Ti_3C_2T_x$ MXenes exposed to HaP precursor solutions, we demonstrate that the surface of $Ti_3C_2T_x$ flakes can be selectively functionalized with either MAI or Pb cations. Interestingly, while $Ti_3C_2T_x$ – Pb interaction may lead to undesired MXene oxidation, MAI provides the passivating effect. We confirm the preference of MAI and Pb adsorption onto =O termination groups with respect to –F, and thus we selectively tune the adsorption strength by using $Ti_3C_2T_x$ MXenes enriched with =O and –F T_x, respectively. Finally, by utilizing the passivation behavior of MAI we show two distinct MAI-concentration dependent effect: (i) MAI-assisted stabilization of $Ti_3C_2T_x$ colloids in organic solvents; and (ii) MAI-assisted inhibition of MXene oxidation and degradation in the solutions. These effects combined allow us to gain active control over the chemistry of MXene-HaP interface in a composite film, while providing chemically-robust and durable MXene-HaP inks, which is an essential step forward towards reliable and adjustable MXene-HaP systems.

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Can we crystallize $BaZrS_3$ at device-compatible temperatures from sulfide precursor films?

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$BaZrS_3$ is an attractive photovoltaic absorber due to its high absorption coefficient (~10^5 cm^{-1}), a band gap of 1.9 eV compatible with Si tandem solar cells, and a benign, non-toxic composition. However, the sensitivity of $BaZrS_3$ to defects and grain boundaries[1] makes the fabrication of high-quality films at device-compatible temperatures (<600 °C) a great challenge.

Recent reports indicate that post-annealing in high sulfur concentrations can yield crystalline films at temperatures as low as 400 °C. However, this moderate-temperature synthesis often relies on solution-based methods or metallic Ba-Zr films, which are highly sensitive to oxidation.[2–5] Today, these methods yield films with poor morphology and residual contamination. As a result, photoluminescence (PL) reports of such films are scarce and indicate poor film quality.[6]

In this study, we use reactive co-sputtering of metallic targets to deposit amorphous metal sulfide precursor films, followed by post-sulfurization at 600 °C. Using amorphous metal sulfide precursor films, we developed a robust synthesis route that allows storage of precursor films for months in the glovebox before post-annealing. We also examine the threshold of oxygen that can be present during our synthesis, demonstrating that it is not necessarily destructive to the film quality.

This synthesis route yields intrinsic, crystalline $BaZrS_3$ films with X-ray diffraction peaks of comparable width to those synthesized at 900 °C and higher. The films also exhibit photoconductivity and distinct PL aligned with the optical absorption onset, indicating a bandgap of 2 eV. These results suggest that sulfide precursors offer a scalable, clean, and more robust alternative for higher-quality chalcogenide perovskite thin films.

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How Halide Perovskites Expanded the Frontiers of Photovoltaic Solar Energy

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Abstract

The discovery of halide perovskite materials as exceptional solar-absorbing semiconductors stemmed from the drive to develop more stable, all-solid-state dye-sensitized solar cells. What began as a modest goal led to far more than anticipated, resulting in the emergence of a remarkable new class of photovoltaic devices. Three-dimensional (3D) and two-dimensional (2D) halide perovskites have become standout semiconductors in recent years, known for their excellent carrier lifetimes and structural adaptability. Yet, the roles of Pb^{2+} and Sn^{2+} ions, along with the impact of organic spacer cations on structure and performance, remain areas that demand deeper investigation. Meanwhile, perovskitoids, a related but structurally distinct class of materials, offer expanded design flexibility through even richer structural and compositional diversity. Recent studies have shown that certain organic cations can stabilize these frameworks effectively. This presentation will explore the latest findings on structure–property relationships in halide perovskites and perovskitoids, providing practical insights into the rational design and integration of organic spacers in crystalline semiconductors and optoelectronic devices.

From Polarized Light to Pressure Sensing: Exploring Multifunctional Hybrid Perovskites

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Recent discoveries have revealed a breakthrough in the field using inorganic-organic hybrid layers called perovskites as the light harvester in the solar cell. The inorganic-organic arrangement is self-assembled as alternate layers, being a simple, low-cost procedure. These organic-inorganic hybrids promise several benefits not delivered by the separate constituents.

In this talk, I will present several topics related to hybrid perovskite synthesis and device applications. I will discuss our recent results on 2D chiral perovskites and their functionality in solar cells and light-emitting diodes (LEDs), demonstrating polarized emission. Additionally, I will present our ability to achieve semi-transparent perovskite solar cells in a variety of colours, independently of the perovskite bandgap.

Beyond their use in photovoltaics, metal halide perovskites exhibit intrinsic piezoelectric properties arising from polarization and the breaking of centrosymmetry in PbX_6 octahedra. In this part of the talk, I will outline our recent investigation into the piezoelectric response of quasi-2D perovskites. Using piezo-response force microscopy, we characterized their behaviour and demonstrated their potential for integration into pressure-sensing devices.

How miraculous are halide perovskites (for PV)? A tale of fables & facts

David Cahen and Gary Hodes Weizmann Institute of Science

Often in research reports or presentations and in public discourse on Halide Perovskites (HaPs) and especially, the solar cells, based on them, ideas were taken as "facts", if facts described as unique, outstanding or the like. This can be problematic if done with insufficient experimental evidence or if common assumptions, used to arrive the conclusion, should be questioned. The latter is the case at least in the Pb-HaPs (referred to from now on as HaPs, excluding Sn-based and double halide perovskites).

An early example is that of "high" mobilities, likely in the initial excitement about the re-discovered treasure. The mobility is fine, enough for solar cells, relatively simple devices. Amazingly the mobilities' temperature dependence that does show a special feature was not noted.

We will touch on other properties, such as lifetime, diffusion lengths, (in)stability, optical absorption, crystal structure from diffraction, and then the centre piece, the *dynamic lattice* which leads to self healing, defect tolerance, defect and dopant densities.

Any material, new for device applications, presents challenges. By mixing fact with fables, we make meeting those challenges that much more difficult.

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Using bond characteristics to predict self-healing properties in materials for sustainable energy conversion

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The long-term sustainability of materials, used for energy generation and storage, highly depends on their ability to self-heal from mechanical and thermal damage. Self-healing of materials occurs through a mass transfer inside the lattice that drives the healing process through two main mechanisms. Either by kinetically stabilized defects in a 'static lattice' ('class I'), or through thermodynamically stabilized defects in a 'dynamic lattice' ('class II'). Although self-healing materials are very important in many applications, there are no clear physical or chemical guidelines for self-healing in materials that can be used to predict their self-healing mechanism.

In this research we use a data-driven approach to find bond character parameters that may affect the mechanism in known self-healing semiconductors. We do this by data mining four parameters: deformation potential (DP), relative structural polarizability (RSP), Pauling's ionicity, and microhardness. Statistical analysis of the data and matching the obtained trends with known theory result in a clear definition of the two mechanism classes based on DP and RSP. Furthermore, by ionicity and microhardness, an improved understanding of the difference between the bonds in class II materials and the defect-informed nature of class I materials is achieved. Our results present important steps in the understanding of the self-healing process, which can direct the search for sustainable self-healing materials for energy uses.

Opportunities and challenges for organic and perovskite photovoltaics in space applications

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Perovskite solar cells (PSCs) and organic solar cells (OSCs), with certified power conversion efficiencies surpassing 27% and 20% respectively, have emerged as promising candidates for space applications due to their exceptional power-to-weight ratios and inherent radiation tolerance. However, their viability depends on overcoming the extreme stresses of the orbital environment, including intense ionizing radiation, severe thermal cycling, and prolonged ultraviolet (UV) exposure.

This presentation details our systematic evaluation of PSC and OSC stability under simulated space conditions. We assessed the radiation hardness of flexible devices using gamma rays, high-energy electrons (0.5–8.5 MeV, fluences up to 10^{16} e/cm²), protons (18 MeV, fluences up to 10^{15} p/cm²), and neutrons (2 MeV, fluence 10^{14} n/cm²). Additionally, we investigated device photostability under UV light and resilience to thermal cycling between +80°C and –85°C.

To elucidate degradation mechanisms, we subjected selected absorber materials and full multilayer stacks to the same stressors and analyzed them with a suite of complementary characterization techniques. Our findings confirm that both PSCs and OSCs exhibit promising stability for prolonged operation in low Earth orbit, withstanding radiation doses equivalent to decades of exposure. We discuss the dominant degradation pathways identified and propose targeted strategies to further enhance device resilience for future space deployment.

This work was supported by Ministry of Science and Higher Education of Russian Federation (Project № 075-15-2024-532).

Bifacial photovoltaic micro-concentrators for space

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Abstract

The key criteria for solar photovoltaic (PV) power in space are distinct from terrestrial applications. Ultra-compactness, maximal *specific* power (kW/kg and kW/m^3), liberal optical tolerance, ease of fabrication, adequate heat rejection, tractable prices, and resilience under cosmic radiation are paramount. These considerations prompted the recent development of PV micro-concentrators.

Here, we present and evaluate new ultra-compact, high-performance micro-concentrators for *bifacial* cells, in particular perovskites, which can attain concentration levels of tens of suns at the relatively large optical tolerances required in space. These designs can be tailored to a desired balance of concentration between the two sides of the bifacial cell at acceptably homogeneous flux distributions. A subsidiary incentive for concentration is cell efficiency increasing linearly with Log(*Concentration*) at low series resistance.

Perovskite PVs are already being tested in space and their deployment in concentrators is under investigation. The simplicity and variety of cell materials create the prospect of bifacial cells that can heighten PV efficiency. We show how our new designs for micro-concentrators for *bifacial* perovskite micro-cells can satisfy the principal figures of merit for PV in space, most notably ultra-compactness (aspect ratios not exceeding 0.4, with total array depths well below 1 mm), large acceptance half-angles reaching 10°, intercept factors up to 0.9, acceptably uniform flux distributions, and concentration values as high as 50.

Towards a More Sustainable Processing of Metal Halide Perovskites

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In recent years, remarkable progress has been made in the field of perovskite solar cells, resulting in power conversion efficiencies (PCE) that surpass 26%. As the vast majority of research efforts are dedicated to their processing from solution, the use of the highly toxic, yet ubiquitously used, dimethylformamide (DMF) for the processing of perovskite represents a major hurdle for their adaptation in industrial applications on the large-scale. In the first part of this talk, I will propose a strategy for selecting green alternatives to DMF that enable a more sustainable processing of perovskite based solar cells. In the second part of the talk, I will introduce novel strategies for a solvent-free fabrication of perovskites by vapor deposition, focusing on addressing the current challenges of this deposition method.

Outdoor Evaluation of Bias-Dependent Performance Dynamics in Perovskite Solar Cells

Amit Kumar and Iris Visoly-Fisher

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Abstract

The stability and degradation of perovskite solar cells (PSCs) are strongly influenced by their electrical operating conditions, with several degradation pathways being partially or fully reversible under light/dark diurnal cycling. Applying an external electrical bias during the night is expected to modulate ion migration causing extraction barriers at the transport interfaces. Building on this understanding, this ongoing study investigates how controlled electrical biasing during both daytime operation and nighttime 'rest' affects the outdoor stability of PSCs.

Three identical perovskite-based NIP solar cells were mounted outdoors for long-term operational monitoring under the following conditions: (i) Maximum Power Point (MPP) tracking throughout day and night, (ii) 0.8 V bias applied during the night alongside daytime MPP tracking, and (iii) –0.4 V bias applied during the night with daytime at MPP tracking. Performance evaluation was performed by estimating using T80 and T50 (time taken to reach 80% and 50% of the initial power conversion efficiency, respectively) lifetime metrics. Although all devices exhibited similar degradation behavior up to T80, estimated T50 values display differences in devices with night time bias compared to devices without it. To gain deeper insights into the recovery mechanisms, impedance spectroscopy, Transient Photovoltage (TPV), and Transient Photocurrent (TPC) measurements are performed and compared for devices before and after outdoor exposure.

Aquavoltaics: Synergy of aquatic photosynthetic bioreactors and perovskite solar cells

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Abstract:

One of the advantages of halide perovskite-based solar cells (PSCs) is that it can be manufactured in a semi-transparent state of varying thickness and color. The semi-transparent PSCs (ST-PSCs) can act as a filter to control the amount and wavelength of photons for photosynthesis. Here, ST-PSCs transparent in the range of 600-700 nm were coupled with a cyanobacteria-containing photobioreactor (PBR) to convert solar energy to electricity and cyanobacterial biomass. Glass-on-glass encapsulated triple cation mixed halide perovskite films (termed 'half cells') of varying thickness and transparency were prepared on FTO substrates. Encapsulated full cells of NIP architecture FTO/c-TiO2/m-TiO2/Perovskite/Spiro/Au were mounted on the PBR and connected to maximum power point tracking. It was found that the cells mounted on the PBR demonstrated longer lifetime compared to the control cells mounted on a static platform, due to the cooling effect of the PBR. This work therefore showed that PSC-PBR coupling increased photovoltaic energy yield as well as aided cyanobacterial growth.

Influence of Carrier Solvents and SAM based Hole Transport Layers on the Performance of Double Cation Perovskite Solar Cells

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The performance of double cation perovskite ($Cs_xFA_{1-x}PbX_3$) based inverted solar cells is strongly influenced by both the carrier solvent systems and the interfacial surface chemistry of the hole transport layer (HTL). In this work, we adopt a less toxic carrier solvent system, N,N-dimethylacetamide (DMAc) and dimethyl sulfoxide (DMSO), and compare it with the commonly used mixture of N,N-dimethylformamide (DMF) **a**nd DMSO to evaluate their influence on perovskite film formation and device performance. Perovskite layers are deposited via a one step spin coating process with controlled antisolvent treatment to set apart solvent-complexation effects on intermediate phase evolution. In parallel, we investigate a new carbazole based self assembled monolayer (SAM) modification (MeO-4PACz) against the MeO-2PACz. Using identical fabrication conditions, we observe that the DMAc based system improves film uniformity and device performance, while the modified SAM enhances interfacial passivation and charge extraction. Overall, the combination of a relatively safer DMAc:DMSO solvent system and MeO-4PACz SAM molecule highlights the importance of synergistic optimization of both solvent chemistry and interfacial layers for a promising route towards efficient and more sustainable perovskite photovoltaics.

Multi-physics Device Simulations of Optimized Semi-Transparent Perovskite Solar Cells: Influence of Material Types and Layer Thicknesses on Transmittance and Electrical Performance

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Abstract

The utilization of perovskite and electrode materials enables the production of semitransparent solar cells that allow partial transmission of light, making them suitable for integration into windows and other transparent surfaces. However, achieving optimal performance is challenging due to the trade-off between transparency and power conversion efficiency (PCE). This study emphasizes the crucial role played by material selection, active layer thickness, and transparent electrode configuration in determining this trade-off in semitransparent perovskite solar cells (ST-PSCs). Through multi-physics device simulations, I optimize the thickness and compare the performance of two active layer materials - $MAPbI_3$ and $CsPbI_3$ - resulting in increased average visible transmission (AVT) as well as PCE. Notably, $MAPbI_3$ outperforms $CsPbI_3$ as an absorber material in ST-PSCs. $CsPbI_3$ achieves an optimal light utilization efficiency (LUE) of 4.06% at a thickness of 300 nm, while $MAPbI_3$ reaches 4.15% at a thickness of 100 nm which shows better performance. Furthermore, my findings demonstrate that the MoO_3/Ag/WO_3 configuration enhances both PCE and AVT compared to alternative configurations due to MoO_3's mitigated parasitic behavior. These results provide valuable insights for advancing solar cell technologies applicable to practical uses such as window integration or other transparent surfaces.

Keywords

semi-transparent perovskite solar cell, Multiphysics simulations, transparent electrode, average visible transmittance, light utilization efficiency

EFFECT OF HOLE TRANSPORT LAYER ON STABILITY AND RECOVERY OF PEROVSKITE SOLAR CELLS

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Abstract:

Perovskite solar cells (PSCs) are known for their high efficiency and low production cost, but one major challenge still limits their use in real-world applications: long-term stability. A key factor that influences this stability is the hole transport layer (HTL), which affects how charges move, how interfaces behave, and how devices degrade over time. The most common organic HTL, Spiro-OMeTAD, performs well initially but degrades quickly because its dopants absorb moisture, evaporate at high temperatures, and react with migrating ions. Inorganic HTLs like copper thiocyanate (CuSCN), on the other hand, are more stable, thermally robust, and do not require dopants, making them a good alternative for durable PSCs. Although CuSCN has shown good indoor stability, very little is known about how it behaves outdoors under sunlight and ambient temperatures.

In this study, we compared the outdoor performance of PSCs made with Spiro-OMeTAD and CuSCN. We fabricated encapsulated triple-cation devices and tested them using J–V, EQE, C–V measurements and long-term maximum-power-point tracking. Early results show that Spiro-OMeTAD devices degrade faster, while CuSCN-based devices maintain more stable performance under heat. However, CuSCN paired with gold electrodes still shows interfacial problems, whereas using carbon contacts leads to much better stability.

A key focus of the ongoing study is to examine whether different HTLs influence potential diurnal recovery behaviour-partial restoration of performance after stress removal-which has been reported in some perovskite systems but remains untested for CuSCN under real outdoor conditions. By analysing both degradation and potential recovery trends, this research aims to uncover the mechanisms limiting durability and provide guidelines for designing more stable, long-lasting PSCs.

LONG-TERM OUTDOOR STUDY OF PEROVSKITE MINI-MODULES IN THE NEGEV DESERT: PRELIMINARY RESULTS AND OPEN QUESTIONS

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Perovskite solar energy materials are a promising choice for the next generation of photovoltaic technology due to their ease of fabrication, tunability of opto-electronic properties, and power conversion efficiency (PCE), which has already reached the level of well-established photovoltaic technologies**.** However, stability and field reliability are the bottlenecks for their commercialization. Addressing these challenges requires a systematic understanding of real-world outdoor performance, yet comprehensive analyses of diurnal metastability, irradiance, and temperature dependence remain limited. Here, we report the outdoor performance of perovskite mini modules deployed under maximum power point (MPP) tracking in the Negev Desert. Results from periodic I-V and MPP measurements identified a daily metastability pattern, where samples exhibit performance degradation overnight, followed by a recovery during the daytime. Analysis of irradiance dependence and diurnal performance shows that PCE trends primarily follow the Fill Factor (FF). Specifically, samples with high series resistance (R_S) exhibited a reduction in PCE and FF under increasing irradiance due to resistive power losses. In contrast, low R_S samples irradiance, exhibiting "ideal" solar cell behavior, with FF increasing with irradiance, driven by the open-circuit voltage gains. Long-term monitoring (120 days) demonstrated divergent aging behavior, ranging from stable performance to initial burn-in followed by partial recovery. Our findings underscore the critical role of minimizing series resistance to maximize outdoor energy yield and enable reliable large-scale deployment.

The authors acknowledge the groups of Dr. Aranzazu Aguirre (from IMEC) for producing the mini-modules and Dr. Maria N. Hadjipanayi (from the University of Cyprus) for the help in the experiment planning. Eventually our results will be compared with the parallel outdoor measurements performing in Germany (Freiburg) and Cyprus.

PHOTOLYUMINESCENCE OF PEROVSKITE SOLAR CELLS OPERATING UNDER LASER AND CONCENTRATED SUNLIGHT ILLUMINATION

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This study was motivated by our development of perovskite solar cells (PSCs) for space applications, which are expected to operate effectively under concentrated sunlight. PSCs could exhibit significant advantages specifically for space, subsuming their resilience to cosmic radiation and the ease of fabrication of micro-cells for ultra-compact micro-concentrators capable of high specific power [1].

We present experimental results of light intensity dependence of PSC power conversion efficiency (PCE) under a wide range of solar concentrations and temperatures. We have concluded that PCE under high light intensity is limited mostly by losses in short-circuit current, indicating considerable bimolecular combination in short-circuit conditions. By parallel measurement of voltage-dependent photocurrent and photoluminescence (PL) under both laser and concentrated sunlight illumination [2], we have confirmed considerable photoluminescence in short-circuited PSC. Possible mechanism(s) of the effect and pathways of its suppression are discussed. The latter is necessary for increasing PSC efficiency under high light intensity.

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Title: Architecture-Driven Outdoor Stability Dynamics in Perovskite Solar Cells

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Abstract:

Understanding how device architecture governs outdoor operational stability is essential for advancing perovskite photovoltaics toward durable field deployment. In this work, we present a rigorous, architecture-controlled outdoor study comparing n–i–p and p–i–n perovskite solar cells. Both architectures were fabricated with the same perovskite absorber, the same encapsulation strategy, and were operated under identical environmental conditions in side-by-side field exposure during both summer and winter. This uniquely controlled configuration enables a direct assessment of architectural influence on real-world stability, independent of absorber chemistry.

Distinct early-time operational responses were observed between the two architectures. p-i-n devices retained a substantially higher fraction of their initial performance during the onset of outdoor exposure, an effect reflected in consistently higher T_{80} values across seasons (459 hours during summer time and > 1000 hours during winter). By contrast, n-i-p devices exhibited a steeper initial decay, indicating a stronger susceptibility to early transient losses under fluctuating outdoor illumination, leading to a T80 of just 86 hours during summer time and 180 hours for winter.

Remarkably, after this initial divergence, the long-term stability pathways of both architectures converged. The performance evolution in the stabilized regime proceeded at nearly indistinguishable rates, leading to T_{50} lifetimes that were closely aligned for both
configurations. These results demonstrate that the dominant architectural differentiation lies in the early operational phase, whereas the intrinsic long-term outdoor robustness of n-i-p and p-i-n devices becomes comparable once transient effects subside.

This work establishes a clear, architecture-resolved understanding of outdoor stability and provides a strong experimental foundation for evaluating perovskite photovoltaic durability under realistic operating conditions.

All Inorganic CsPbI3 Solar Cells

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Abstract

All-inorganic perovskite solar cells based on $CsPbI_3$ have emerged as one of the most promising photovoltaic technologies due to their exceptional optoelectronic properties and their potential for superior thermal stability compared to hybrid organic–inorganic perovskites. $CsPbI_3$ possesses an ideal bandgap (~1.7 eV), high absorption coefficient, and long carrier diffusion lengths, making it a strong candidate for high-efficiency single-junction devices as well as tandem applications. The absence of volatile organic cations further offers the prospect of enhanced operational durability under heat and ambient conditions, addressing one of the major limitations of current perovskite solar cells. However, despite these advantages, the practical application of $CsPbI_3$ is hindered by several intrinsic challenges. The most significant is the material's strong tendency to convert from the photoactive black α-phase to the non-perovskite yellow δ-phase at room temperature. This phase instability severely limits both efficiency and long-term reliability. Additionally, $CsPbI_3$ films often suffer from high defect densities, poor surface passivation, and suboptimal interface alignment, all of which contribute to non-radiative recombination and reduced charge extraction. Achieving uniform, dense, pinhole-free films with controlled stoichiometry is also complex, as slight deviations in precursor chemistry or crystallization dynamics can dramatically affect phase purity and device performance. This work aims to address these limitations by investigating compositional control, additive engineering, and optimized processing conditions to stabilize the black phase during and after film formation. In parallel, surface and interface engineering strategies are employed to minimize trap states, improve carrier transport, and enhance environmental resilience. By systematically studying these factors, the goal of this research is to achieve $CsPbI_3$ solar cells that combine high power-conversion efficiency with meaningful operational stability. This poster presents the motivation, challenges, and experimental approaches guiding the development of robust all-inorganic perovskite photovoltaics suitable for practical deployment.

Fully Printable Inorganic Perovskite Light Emitting Diodes in the Visible Region

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Abstract

Stable perovskites light sources with long-term operational durability are essential for future commercial applications. This work presents ongoing research toward a fully printable and entirely inorganic mesoporous indium tin oxide (ITO) perovskite light-emitting diode (ITO-PeLED) operating in the visible range. The deposition of $CsPbBr_3$ into mesoporous ITO is investigated, with the goal of optimizing crystal formation and charge injection to enhance LED performance. Preliminary devices exhibit green electroluminescence (EL) centered at approximately 524 nm, with an initial external quantum efficiency (EQE) of 0.01%, which continues to improve through ongoing process optimization. Additionally, the same devices were tested as solar cells, achieving a power conversion efficiency (PCE) of up to 1.2%. These results highlight the potential of this architecture for the development of efficient, stable, and scalable PeLEDs for future large-scale manufacturing.

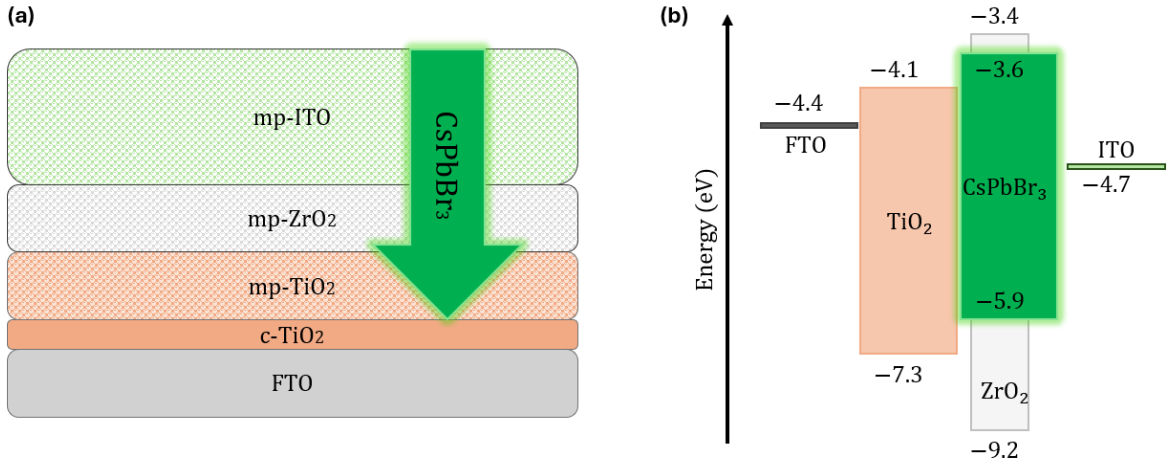

Fig. 1

(a) A schematic illustration of the ITO-PeLED structure. (b) Energy-level diagram of the different layers in the structure.

Outdoor stability of Spin-coated vs Slot-die coated organic photovoltaic devices

Flavia Pazhayattil[1], Eswaran Jayaraman[2], Sambathkumar Balasubramanian[2], Hsuan-Yu Wang[2], Morten Madsen[2], Vida Engmann[2], Daniel Garcia Martos[2], Iris Visoly-Fisher[1]

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Abstract:

The long term stability of non-fullerene absorber-based organic photovoltaic (OPV) devices under real outdoor conditions is essential for advancing their commercial viability. In this study, we evaluated the real-world photostability of encapsulated PM6:Y7-12 devices fabricated by spin coating or slot-die coating techniques and tested under desert conditions with and without a UV filter. Devices were monitored on a two-axis solar tracker under maximum power point conditions for up to 78 days during spring, summer, and fall, exposing the devices to strong fluctuations in irradiance and ambient temperatures between 25 - 40 °C.

Slot-die-coated devices consistently exhibited longer operational lifetimes than spin-coated devices. Analysis of pre-exposure and post exposure JV characteristics revealed that in degraded devices, the dominant loss mechanism was fill-factor decay (~50%), indicating severe charge-transport degradation, while Jsc and Voc decreased more moderately (10–20%). The stable slot die coated devices (with UV filter) showed minimal loss in Jsc and ~25% FF loss. Our results demonstrate that (1) slot-die coating yields intrinsically more stable BHJ morphology compared to spin-coating devices, and (2) UV exposure is a stronger degradation driver than temperature under desert outdoor operation. These findings provide important insights for scaling OPV manufacturing and for designing outdoor-relevant stability tests.

A perovskite- hematite photovoltaic-photoelectrochemical tandem integrated system for outdoor testing

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Abstract

Green hydrogen production enables the use of hydrogen as a mean of renewable energy storage. One of the paths toward green hydrogen production combines photovoltaic-photoelectrochemical (PV-PEC) technologies, in which the PV power yield is used for driving PEC water splitting. A hybrid, tandem such device utilizes solar energy for both processes without increasing the spatial footprint. The challenges of such coupling include current matching, spectral mismatching and PV high photovoltage to drive water splitting reaction. Hematite (Fe3O2) is a promising PEC photoanode due to its relatively high stability and suitable bandgap for partial solar spectrum absorption. Perovskite solar cells are good candidates to be integrated with PEC due to the bandgap flexibility afforded by different perovskite compositions. Most of the PV-PEC systems demonstrated hitherto were characterized in lab conditions only.

The aim of this study is to characterize the outdoor performance of an integrated tandem PV-PEC system with a semitransparent perovskite-based PV device and a hematite photoanode-based PEC cell, and understand its dependence on the daily varying solar radiation spectrum, irradiance, and ambient temperature. An experimental cell was designed to allow testing of different configurations such as the PV cell position in front of or behind the PEC cell. Initial outdoor tests were performed. Understanding the behavior of this PV-PEC tandem system in outdoor conditions will enable optimization of the choice of bandgap of the perovskite solar cell for current and spectrum matching, towards improved solar to hydrogen efficiency.

PV in Tigray

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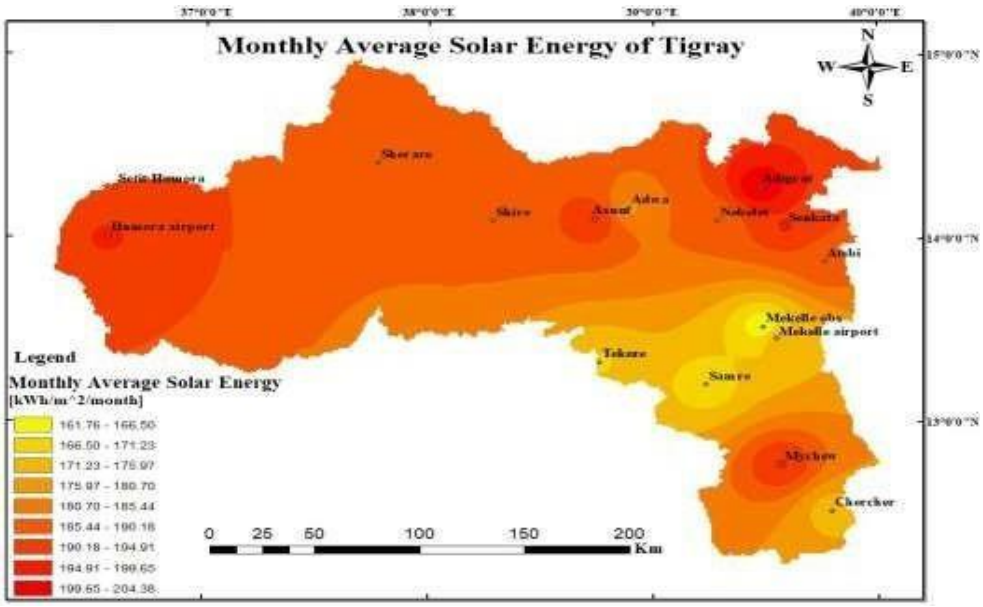
Abstract

Availability of properly analyzed energy resource potential data is a prerequisite in energy planning and development. However, this was hardly applied in Ethiopia's renewable energy turnkey project development strategies. The study of this paper focuses on devel-oping solar energy resource map of Tigray to accelerate the expansion of solar energy to improve electricity access through on-grid and off-grid development schemes. This study uses monthly sunshine hours data of sixteen meteorological stations measured at 2m and average yearly solar radiation data of twenty-two satellite stations validated by three sites' solar radiation data measured at 10 and 30m height. The solar energy potential was analyzed by taking relevant atmospheric and meteorological factors to produce solar radiation components. Accordingly, average annual solar radiation of Tigray was found to be 6.1kWh/m2/day and 5.3 kWh/m2/day based on meteorological and satellite data respectively. The meteorological result gave a closer estimate to Ethiopia's ESMAP global solar Atlas result of 5.83 kWh/m2/ day. Finally, monthly and annual average solar radiation maps of the region were developed by using GIS. The study's result would contribute to assisting different solar energy developers to prepare better solar energy development planning in alleviating the chronic energy poverty of the region.

Keywords: Renewable Energy; Sunshine Hour; Solar Energy Resource; Solar Radiation Mapping.



Effect of Sn_xN_y passivation layer on SnO2 electron transport layers in halide perovskite solar cell

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Tin oxide (SnO_2) thin films are highly favored as electron transport layers for perovskite solar cells, owing to high electron selectivity and conductivity, as well as transparency and chemical stability. Compared to the traditional titanium dioxide (TiO_2) thin-films that require high-temperature processing, SnO_2 could be easily coated using various low-temperature processes such as CVD (chemical vapor deposition) or ALD (atomic layer deposition) and magneton sputtering, offering the added advantage of compatibility with flexible substrates. However, SnO_2 thin films suffer from interfacial defects such as oxygen vacancies, Vo, and the presence of surface hydroxyl groups (Sn–OH). Oxygen vacancies may cause trap states that lead to charge recombination in solar cells, reducing efficiencies, while hydroxyl groups react with the perovskite layer leading to degradation.

Here, we present a mitigation strategy to impede the adverse interfacial defect effects using tin nitride as a passivation layer. In this study we fabricate SnO_2 thin films using reactive RF magneton sputtering at room temperature in the presence of O_2, while the Sn_xN_y is deposited via reactive sputtering of a metallic Sn target in an Ar/N_2 mixture. By carefully controlling the gas partial pressures we are able to tune the types of layers we obtain. The layers are characterized by XPS (X-ray photoelectron spectroscopy, XRD (X-ray diffraction), and SEM) scanning electron microscopy) to analyze the layers by providing information on their characteristics. Initial investigation on full n-i-p perovskite cells show that Sn_xN_y passivated SnO_2 improves device stability and efficiency. Our bilayer approach will enhance the efficiency and stability of the perovskite solar cells in the n-i-p architecture, leading to possible large-scale implementation for a renewable energy-based future.

Suppressing Radiation-Induced Degradation in Lead Halide Perovskites via Material Engineering

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Perovskite solar cells (PSCs) offer an exceptional combination of high efficiency, low-cost fabrication, high specific power, and superior radiation resistance, making them attractive for both terrestrial and space applications. However, their operational stability under extreme conditions remains a critical challenge. While molecular modifiers are widely used to improve the efficiency or stability of PSCs against terrestrial degradation factors, their influence on perovskite stability in space environments has been largely unexplored and requires thorough investigation.

Our recent studies have demonstrated that gamma rays (1–2 MGy) trigger significant structural degradation in multication perovskite films, including $(CsFA)PbI_3$ and $(CsMAFA)PbI_3$ (where MA^+ and FA^+ denote methylammonium and formamidinium cations, respectively). These materials undergo radiolytic decomposition, resulting in the formation of PbI_2 and metallic lead (Pb^0). Furthermore, we observed pronounced phase segregation in multication compositions, resulting in localized regions resembling $MAPbI_3$, $FAPbI_3$, and $CsPbI_3$ phases.

Given the essential role of multication perovskites in state-of-the-art photovoltaic devices, we targeted the enhancement of their radiation hardness, focusing on $(CsMAFA)PbI_3$ systems. We demonstrated that rationally designed modifiers significantly improve the radiation hardness of perovskite absorber films against high-energy electrons, protons, neutrons and γ-rays by simultaneously suppressing radiolytic decomposition and phase segregation.

Our findings demonstrate that targeted molecular design can effectively suppress key radiation-induced degradation pathways in lead halide perovskites and boost the operational stability of perovskite solar cells under harsh space conditions and terrestrial high-radiation environments.

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Investigation of Terminated Mxenes for Interface Engineering in Perovskite Solar Cells: A DFT Study

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Perovskite solar cells (PSCs) have rapidly emerged as a leading third-generation photovoltaic technology due to their high power conversion efficiencies, tunable optoelectronic properties, and low-cost, solution-processable fabrication. By taking advantage of the versatile ABX_3 perovskite structure, these devices have achieved efficiencies approaching 30 percent through careful compositional tuning, particularly in mixed organic-inorganic and mixed-cation formulations. Despite this progress, challenges such as long-term instability, interfacial defects, and charge recombination continue to limit device performance and durability, prompting the search for more effective interlayer materials. MXenes, which are two-dimensional transition-metal carbides, nitrides, and carbonitrides, possess highly adjustable surface chemistries that can enhance conductivity, promote defect passivation, improve energy-level matching, and increase environmental stability. In this work, we present a comprehensive density-functional-theory (DFT) investigation of Ti_3C_2 with various surface terminations including O, OH, F, Cl, Br and I, enabling controlled alignment with perovskite and charge-transport layers to support efficient carrier extraction and reduced interfacial recombination. Our study examines their work functions, formation energies, and structural distortions, followed by an analysis of perovskite and MXene interfacial properties and the potential of these materials to improve the performance and stability of next-generation PSCs.

Broadband Lossy Waves at Ultrathin Metals Interface for Solar Photothermal Conversion and Water Desalination

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Interfacial solar photothermal conversion for water desalination is an efficient and sustainable method for producing clean water, in which sunlight absorbed at the water-matter interface generates localized heating and rapid evaporation with minimal thermal losses. By concentrating heat only at the evaporation surface, this approach offers higher energy efficiency and simple off-grid operation. Effective performance relies on photothermal materials with strong absorption, low reflectance, and high surface area.

Recently, we explored broadband lossy waves excited through a prism at ultrathin metal films as a method for solar water desalination. Here we report on the use of porous silicon (PSi) coated with ultrathin absorbing metal (12nm Ni) as a platform for efficient photothermal conversion. PSi is well suited for this purpose due to its highly porous structure, which enhances photon trapping, increases optical absorption, and promotes multiple internal scattering. Its graded refractive-index transition from silicon to air further suppresses reflectance, enabling efficient photothermal conversion and strong heat localization.

PSi samples were fabricated by electrochemical etching under various current densities to tune porosity and optimize photothermal behavior. Initial evaporation tests showed that a 12 nm Ni coating on PSi etched at 550 mA achieved an evaporation rate roughly 1.8× higher than smooth silicon.

[1] Aideen Shlebe, I. Abdulhalim, *JOLT* 187, 112838 (2025).

Quantum Cutting Pathways in Halide Perovskites: Mechanistic Insights for Next-Generation High-Efficiency Solar Cells

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The global transition toward sustainable energy relies also on improving the efficiency and performance of solar-cell technologies. However, conventional solar cells are limited by the Shockley-Queisser conversion efficiency ceiling of ~33%, in part because high-energy photons from the blue solar spectrum lose excess energy as heat through thermalization before electrical conversion (one of the S-Q model's assumptions).

Quantum cutting (QC) presents a promising approach to convert a high-energy photon into two lower-energy ones, so as to go beyond the S-Q model. Thus, in rare-earth-doped systems, a single high-energy photon excites the host lattice and can transfer energy to several types of rare-earth ions (e.g., Yb^{3+}), each emitting lower-energy photons. When integrated with halide perovskite absorbers, this process could generate internal quantum efficiencies exceeding 100%.

This work investigates optimal conditions for quantum cutting in halide perovskites and elucidates underlying mechanisms. Our model system, $Yb:CsPb(Cl_{0.6}Br_{0.4})_3$, exhibits characteristic photoluminescence (PL) in both the blue region (perovskite) and near infra-red (NIR) region (Yb^{3+}), enabling direct observation of the QC process. We fabricated thin films via spin-coating with varying Yb^{3+} concentrations and annealing parameters. Using time-resolved PL measurements, we determined PL decay lifetimes in both spectral regions and identified optimal conditions that minimize non-radiative losses. Higher Yb^{3+} concentrations combined with lower annealing time and temperature reduced the non-radiative loss fraction. Notably, PL lifetime analysis revealed previously unreported QC behavior, including biexponential NIR-PL decay, suggesting two distinct Yb^{3+} sites and more complex mechanisms than initially hypothesized. These mechanistic insights provide a foundation for rational design of quantum-cutting-enhanced perovskite solar cells.

Impact of a chiral-centered barrier molecule on the piezoelectric response of quasi-2D Perovskites pressure sensors

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2D perovskites can exhibit the piezoelectric effect, in which a material can generate an electric field due to a spatial distortion of the crystal lattice (piezoelectric response). Due to this property, 2D perovskites are considered prime candidates for pressure sensors. The spatial distortion in 2D perovskites highly depends on the barrier molecules used and the "n" value of the 2D structure (n=the number of perovskite layers confined between barrier molecules). Currently, the piezoelectric response in 2D perovskites pressure sensors yields a low current (μA region).This study focuses on improving the piezoelectric current by introducing the (1R,2R)-(+)-1,2-Diphenylethylenediammonium (1R,2R-DPEDA) molecule, a double chiral-centered organic molecule, as a barrier in the 2D structure. The chiral centers act as symmetry-breaking hotspots, increasing the distortion and the overall polarization in the lattice, thus increasing the piezoelectric current yield.

Understanding the Halide Perovskite Composition Effect on Self-healing

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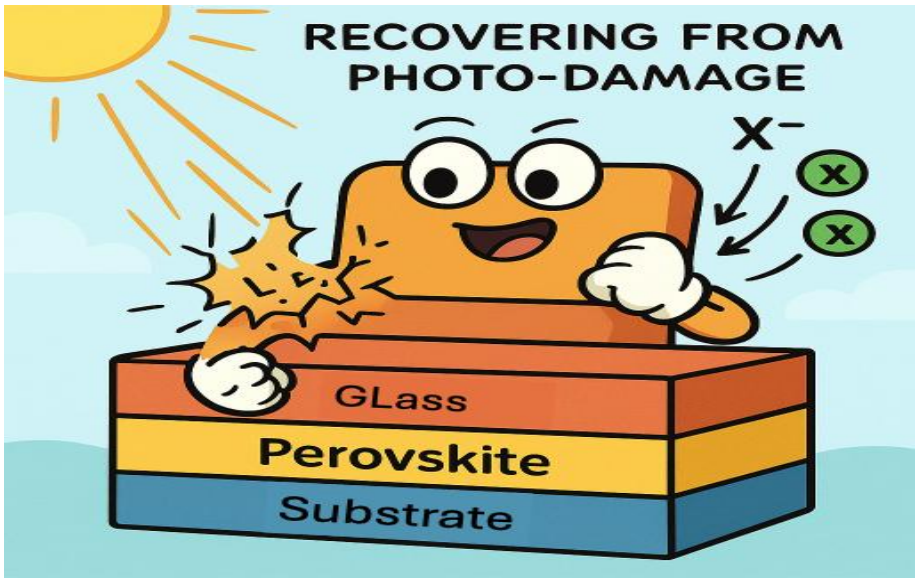
Self-healing of damage in halide perovskite (HaP) materials has the potential to greatly ameliorate stability issues in HaP devices. While previous studies have predominantly explored single-cation perovskites, we report on self-healing dynamics in thin HaPs films, the form in which HaPs are used in solar cells, to try to optimize self-healing in these. Under strong luminescence, thin films of single-cation, double-cation, and triple-cation mixed halide perovskite exhibit varying degrees of healing. Among them, the triple cation mixed halide composition exhibits superior self-healing properties. The dynamics are critical, as self-healing must be fast enough to prevent permanent damage due to excessive damage accumulation. We employed two complementary techniques—Fluorescence Recovery After Photobleaching (FRAP) and Photoluminescence imaging—to monitor the healing process in polycrystalline thin films after photo-damage using high-power LASER.



2D-3D perovskite heterojunctions using vapor phase dual cation exchange

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Hybrid lead-halide perovskites have emerged as one of the most promising materials for photovoltaics due to their remarkable optoelectronic properties. However, the poor environmental stability of perovskites remains a major obstacle to commercialization. Perovskites that are two dimensional (2D) overlayed on the surface of the light absorbing three dimensional (3D) perovskites are used to improve the stability and the performance of the perovskite solar cells. The dimensionality of the 2D perovskite layer plays an important role in the performance of solar cells. Tailoring the dimensionality of the 2D perovskite overlayer can improve both performance and stability.

Here we present a vapor phase dual cation exchange method that we developed to tune the dimensionality of the 2D perovskite layer from an n=1 phase to a mixed up to n=6 phase, at room temperature. This is achieved by exposing the surface of the 3D perovskite layer to controlled amounts of methylamine (MA) and 4-fluoro phenethyl ammonium (FPEA) vapors. By carefully controlling the ratios of the two amines, an optimal mixed phase 2D perovskite on the surface of the 3D perovskite can be achieved, which has better energy alignment with the 3D perovskite layer as well as improved charge transport properties. The 2D perovskite growth was monitored by an in-situ photoluminescence setup allowing for real-time tracking of the growth dynamics. Improved energy alignment was observed as higher open-circuit voltages and higher fill factors. The 2D solar cell stability was notably higher than pristine 3D perovskite cells. Our dual cation exchange method simultaneously improves the performance and stability of perovskite solar cells, while also being highly scalable for future utilization on large area devices.

The Polybromide Melt (PBM): the key for making and stabilizing Cu, Au, Pb and Sn Halide-Perovskites

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Halide perovskites (HaPs) continue to amaze the materials science and engineering community with their unorthodox materials properties, such as self-healing and/or defect tolerance, that lead to high-quality functional opto-electronic material while keeping a relatively simple and non-demanding solution-based synthesis. On the other hand, they still suffer from high chemical activity, reactivity, and instability in ambient environments and when interacting with layers that surround them. With this in mind, we were asking ourselves, "Is there a common ground that is responsible for both degradation and healing effects, and if there is, can it be isolated and manipulated?" With this in mind, we started exploring the polybromide melt (PBM) several years ago, with the belief that it holds the secret to provoking both healing and degradation.

We will share our most recent understanding of how polybromides, in particular PBM – a mixture between Br_2, MABr (methylammonium bromide), and HBr – are involved in the formation of Pb, Sn, Au and Cu based HaPs. directly from their metallic form. The investigation of the transformation chemistry and additional stability tests reveled the mechanism through which HaPs are formed, stabilized, or de-stabilized. Our findings show that the polybromide result in formation of HaP structures from all the metals, despite fundamental differences in the redox potentials. Using electrochemical reasoning that include disproportionation reaction and polyhalides reduction, we found that the polybromides are crucial for the (de-)stabilization in all these perovskite systems. For example, Sn^{2+} form of the perovskite will have a better tolerance towards oxidation to Sn^{4+} than when adding SnF_2 when little amount of PBM is added, but when excessive, it accelerates the oxidation of Sn to Sn^{4+}.

Overall, we show that understanding of the chemistry of polyhalides is critical for the future implementation of HaP for different applications, in synthesis, and their long-term sustainability.

Enhancing Crystallinity of Halide Perovskite Thin Films via Controlled Mxene Incorporation

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Halide perovskites (HaPs) exhibit advantageous optoelectronic properties including a direct bandgap, a high light absorption coefficient, and long charge-carrier diffusion lengths. These properties position HaPs as leading candidates for high-efficiency photovoltaic technologies. Despite these merits, issues related to long-term operational stability and large-scale manufacturability continue to hinder their practical deployment. MXenes, an emerging class of two-dimensional transition metal carbides and nitrides, have been reported to modulate HaP crystallization kinetics [1], adjust the work function through their surface termination chemistry [2], and improve both power-conversion efficiency (PCE) and device stability in HaP-based solar cells [3].

In this systematic study, we examine how MXene incorporation influences the structural and optoelectronic characteristics of HaP thin films. After deriving the optimal composition and preparation sequence for MXene-HaP precursor solutions we create films that show high reproducibility, notable improvements in crystallinity, morphological uniformity, and enhanced grain size. Steady-state photoluminescence measurements reveal pronounced quenching, indicating the suppression of radiative recombination, which may suggest charge-carrier transition between the HaP to the incorporated MXenes. These insights show that MXenes can act as an effective tunable additive for enhancing the performance and stability of HaP-based solar cells.

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Computational electronic structure analysis of Ru-based vacancy ordered halide perovskites

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Halide perovskites have been examined for their potential attractive electronic properties for photovoltaic applications. However, many promising candidates are known for issues with their stability, limiting their usefulness. In order to expand the available chemical space, a perovskite-derived structure of the form A2B(IV)X6, with Pt-group metals (such as Ru), being common candidates for the B-site. Due to the vacancies in the structure, the octahedra are relatively isolated, and have been experimentally shown to have 0D like properties, such as having magnetic properties. However, some systems, such as the Ru-based ones, lack an appropriate supportive computational backing. In this study, we present a computational analysis of selected Ru-based perovskites, focused on the electronic structure and magnetic properties, using a purely predictive method for structure determination and proper level of theory for the electric structure.

Transient Surface Photovoltage and Photoluminescence Spectroscopy of Semiconductor Materials

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This study presents the development and implementation of a transient spectroscopy platform that simultaneously measures surface photovoltage (tr-SPV) and photoluminescence (tr-PL) to investigate charge carrier dynamics and defect states in semiconductor materials. Tr-SPV tracks the evolution of photogenerated charge separation and relaxation over time, providing insights into carrier transport and surface/bulk/interface states. tr-PL monitors the time-dependent emission from recombining carriers, revealing radiative recombination pathways. By combining these techniques, we obtain a comprehensive view of the overall charge carrier dynamics.

The system utilizes a tunable laser source with a broad wavelength range, enabling precise excitation of different electronic states. A non-contact probe is used to measure the transient response, eliminating the need for physical electrodes and allowing to measure single crystals, powders and thin films. The setup resolves transient carrier rise and decay times from the nanosecond scale to processes occurring over 10 milliseconds, thereby bridging ultrafast and slower dynamics.

As test cases, we will demonstrate how tr-SPV can be a valuable tool to probe charge extraction in Si/Perovskite tandem solar cells under bias light illumination, as well as tr-PL measurements at low pulse repetition rate.

By integrating experimental measurements with drift-diffusion modelling, we plan to analyze charge transport, recombination kinetics, and defect-related processes. This approach allows us to extract key material properties, including charge transfer rate constants and densities of traps at interfaces. The insights gained contribute to a deeper understanding off the different loss mechanisms and charge transfer limitations in high-efficiency solar cell devices, advancing the development of optimized materials.

Many-Body Effects in Lattice Dynamics: A Case Study of the Displacive Phase Transition in $BiVO_4$

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Bismuth vanadate ($BiVO_4$) is a leading photoanode and photocatalyst material for solar fuel and energy conversion, where performance is closely linked to its lattice dynamics. Although $BiVO_4$ remains in its monoclinic phase under typical operating conditions, it undergoes a displacive phase transition to the tetragonal structure at elevated temperatures (~523 K). The strong anharmonicity and mode coupling associated with this transition influence its vibrational and electronic properties well below the critical point. As a result, understanding the effects of incipient structural instabilities is essential for interpreting vibrational spectra and optimizing device behavior at ambient and moderately elevated temperatures.

This work presents a coupling-based dynamical model that embeds interaction terms directly into the lattice equations of motion. Using $BiVO_4$ as a case study, we reproduce key spectral anomalies — intensity redistribution, asymmetric lineshapes, and polarization-dependent snaking — that conventional Lorentzian models fail to capture. These results demonstrate that mode coupling is an intrinsic feature of the dynamics of displacive phase transitions. Our approach links many-body lattice interactions to experimentally observed features, offering a powerful tool for studying anharmonicity and phase transitions in complex materials.

Growing Titanium Oxynitride Electron-Transport Layers by Plasma-Enhanced Pulsed Laser Deposition

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High-efficiency solar cells rely on carrier-selective contacts that suppress recombination and series resistance while remaining optically transparent. Titanium oxynitride (TiO_xN_y), an n-type electron-transport layer (ETL), combines high composition-tunable conductivity, an adjustable low work function, and a wide bandgap, enabling efficient electron extraction. Compared with the benchmark ETL material TiO_2, TiO_xN_y provides these advantages at similar transparency while reducing reliance on oxygen-vacancy–mediated conduction that introduces traps and hysteresis. Ultrathin TiO_xN_y films are grown on FTO-glass by plasma-enhanced pulsed laser deposition (PE-PLD), ablating a TiO_2 target under continuous ion plasma conditions ranging from pure O_2 to pure N_2 with varying O/N ratios to study suitable conditions for incorporating nitrogen into the oxide lattice and transforming it into an oxynitride. In contrast to high-temperature, long-duration ammonolysis, which operates near thermodynamic equilibrium and suffers from reduction of transition metal oxides, limited control over anion stoichiometry, and parasitic phase formation, PE-PLD is a far-from-thermodynamic-equilibrium process that delivers orders of magnitude higher energies (10^3–10^5 meV/atom) compared to chemical-based methods (~25–60 meV/atom), enabling phase stabilization, high purity growth with active nitrogen species, and precise stoichiometric and structural control under low-thermal-budget conditions that suppress unwanted phase transformations. The structural, optical, and electronic properties of the resulting films are characterized by XRD, XPS, and UV-Vis spectroscopy to assess crystallinity, bonding, stoichiometry, band alignment, and optical gap relevant to charge selectivity and transparency. This approach aims to produce phase-pure, low-defect TiO_xN_y films with tunable optical gap and work function, targeting robust electron selectivity and low contact resistivity competitive with widely used oxide contacts.

Accessing Metastable Bi_2O_3 Phases Via Far-From-Equilibrium Processing

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Accessing metastable semiconductor phases with superior optoelectronic properties remains a fundamental challenge in energy materials synthesis. Metal oxides exemplify this challenge, where metastable polymorphs often demonstrate enhanced light absorption, charge separation, and catalytic activity compared to their thermodynamically stable counterparts (e.g., metastable anatase vs. stable rutile TiO_2, metastable hexagonal vs. stable monoclinic WO_3, metastable β- vs. stable α-Bi_2O_3). However, conventional thermal processing methods that lead to thermodynamically stable materials cannot reliably synthesize and stabilize metastable phases due to extended heating durations that promote relaxation toward thermodynamic equilibrium. We use bismuth oxide (Bi_2O_3) as a model system to address this challenge. The metastable β-phase has a smaller bandgap (2.4 eV) compared to the thermodynamically stable α-phase (2.8 eV), offering enhanced visible-light absorption and superior charge transport properties for photocatalytic applications. However, conventional thermal processing cannot access the β-phase due to extended heating durations that allow thermodynamic relaxation to the stable α-phase, preventing kinetic trapping of the desired metastable structure.

We demonstrate Flash Photonic Heating (FPH) as a solution to this synthesis challenge. FPH uses millisecond white-light pulses with ultra-rapid heating rates (10^6–10^7 °C/s) to selectively convert α-Bi_2O_3 to β-Bi_2O_3 while preserving substrate integrity, enabling kinetic control over phase formation. We present X-ray diffraction data confirming complete α-to-β phase transformation in Bi_2O_3 films on FTO substrates. Surface photovoltage spectroscopy shows distinct photoresponse characteristics of the β-phase, consistent with its reduced bandgap and increased visible-light absorption. FPH processing parameters, including pulse duration, energy density, and heating rates, control selective phase formation. This work establishes FPH as a fast, substrate-compatible method for accessing metastable semiconductor phases, offering new opportunities for tunable optoelectronic materials in energy conversion.

Photocatalytic Semiconductor-Metal Hybrid Nanoparticles: From Single-Atom Catalyst to Metal Tips

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Abstract:

Semiconductor-metal hybrid nanoparticles (HNPs) are promising materials for photocatalytic applications such as water splitting, manifesting high efficiencies compared to their individual constituents. Of particular interest are heavy-metal free HNPs, which are environmentally and biologically compatible, and may therefore be utilized to promote a sustainable economy. To this end, heavy-metal free HNPs have demonstrated low photocatalytic yields, especially under visible light, which limits the realization of actual HNP-based applications. Herein, novel HNPs are synthesized in a "single-atom catalyst" (SAC) regime, achieved via deposition of atomic co-catalysts on the semiconductor nanocrystals. This new SAC regime of HNPs, demonstrated first on ZnSe-Au nanorods, exhibits photocatalytic hydrogen generation, with strong dependence on the co-catalyst concentration and a sharp response maximum in the SAC regime. Further chemical and structural characterizations, including atomic resolution electron microscopy, X-ray photoelectron spectroscopy, and X-ray absorption are used to establish the SAC regime. By correlating structural, chemical, and mechanistic studies of the newly discovered SAC regime, and identifying the transition between SACs and the traditional metal-tip regime, we reveal the effect of both the quantity and the nature of the metal sites on the photocatalytic functionality. This holistic view of the intriguing SAC-HNPs will set the stage for designing highly efficient and sustainable heavy-metal free photocatalysts for numerous applications.[1]

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Time-Resolved Surface Photovoltage Under Circularly Polarized Light: Unveiling Giant Chiral Photoresponse in 2D Perovskites

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Introducing chiral organic cations is an effective strategy for inducing chirality in perovskites, leading to crystallization in chiral-polar point groups.[1] This unique structural characteristic not only imparts chirality but also introduces additional functionalities, such as the ability to interact with circularly polarized light [2,3] and exhibit anisotropic charge carrier behaviour. [4] These materials hold great potential for applications in optoelectronics, spintronics, and efficient energy harvesting.

Currently, it is challenging to assess the efficiency of the chirality transfer from the organic chiral molecule to the perovskite, since it requires the construction of a full optoelectronic device with two electrical contacts.

In this study, we adopted a method involving the dynamic long-range organization of 2D (R/S-MBA)$_2$PbI$_4$ chiral perovskites, guided by chiral dopants, which enhances the chiral response [5]. We will discuss their distinct properties, with a focus on the interplay between chirality and charge transport, using a novel approach of time-resolved SPV measurements under a circularly polarized laser beam, without the need to fabricate a whole device, offering direct insights into the role of chirality in these processes. The results revealed differences in charge separation between the R and S enantiomers, manifested as distinct photovoltage responses under right- and left-handed circularly polarized light (RCPL and LCPL). The measurements showed pronounced anisotropic behaviour, with the R sample exhibiting enhanced signals at RCPL and the S sample at LCPL. Furthermore, the calculated g_{SPV} anisotropy factor, which translates to the equivalent photocurrent anisotropy factor (g_{ph}) via the open-circuit law, reveals a giant g_{ph}approaching the theoretical maximum value of 2.

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NC meets CN: Porous photoanodes with polymeric carbon nitride/ZnSe nanocrystals heterojunctions for photoelectrochemical applications

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Abstract

The utilization of photoelectrochemical cells (PEC) for converting solar energy into fuels (e.g., hydrogen) is a promising method for sustainable energy generation. We demonstrate a strategy to enhance the performance of PEC devices by integrating surface-functionalized zinc selenide (ZnSe) semiconductor nanocrystals (NCs) into porous polymeric carbon nitride (CN) matrices to form a uniformly distributed blend of NCs within the CN layer via electrophoretic deposition (EPD). The resulting type II-heterojunction at the CN/NC interface facilitates intimate contact, ensuring stable connections without the need for insulating binders, thus promoting efficient charge separation and suppressing carrier recombination. This unique CN/NC composite structure serves as a photoanode demonstrating a photocurrent density of 160 ± 8 μA cm^{-2} at 1.23 V vs. reversible hydrogen electrode (RHE), 75% higher compared with a CN-based photoelectrode, for approximately 12 hours. Spectral and photoelectrochemical analyses reveal extended photoresponse, reduced charge recombination, and successful charge transfer at the formed heterojunction, providing enhanced PEC oxygen production activity with Faradaic efficiency of 87%. The methodology allows integration of high-quality colloidal NCs within porous CN-based photoelectrodes providing numerous knobs for tuning the functionality of the composite systems, thus showing promise for achieving enhanced solar fuel production using PEC.

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Automated Procedure for *Ab Initio* Calculation of Electron and Hole Mobilities in Organic Semiconductors

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Molecular organic semiconductors frequently exhibit hopping charge carrier mobility described by the Marcus equation. *Ab initio* prediction of the Marcus parameters (reorganization energy, hopping integral, and site energy disorder) necessary for calculating the mobilities is an urgent problem. Existing "cheap and dirty" methods are based on the so-called Energy Splitting in Dimer (ESID), which is basically the splitting of HOMOs (for holes) or LUMOs (for electrons) of the adjacent monomers between which charge hopping occurs. This approach is inaccurate, because the conformation of the molecule with additional electron or a hole differs substantially from the initial (neutral) state. We developed a Linear Synchronous Transit-like approach taking into account large amplitude motions in monomers upon hole or electron migration. Charge migration profile involves the region of quasi-degeneracy, which necessarily requires a multireference treatment. Here we present an automated procedure for building LST points, configuring input files for multireference *ab initio* calculations, and analyzing the outputs to get the Marcus parameters. The procedure is applied to a series of fluorinated thiophene-phenylene oligomers, for which ESID results contradict the experimental observations.