Winter Workshop on Materials for Energy

wWME

2026

BOOK OF ABSTRACT

From January 27th to February 1st 2026
Hotel GrünerBaum
Brixen - Italy

Welcome!

It is with great pleasure that we announce the third edition of the Winter Workshop on Materials for Energy – wWME 2026, to be held in Brixen (BZ), Italy, from January 27th to February 1st.

The program will be composed by a combination of invited and contributed talks, given by established and early-career scientists.

The idea is to create a connection between simulations and experiments in the field of energy harvesting in a friendly atmosphere with lots of space for networking activities.

We look forward to seeing you in Brixen!

The Organizing Committee

Invited Speakers

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AMBIPOLAR TRANSPORT AND DOPING IN HALIDE PEROVSKITES

M. Saba, N. Sestu, S. Matta, A. Bhardwaj, F. Mattana, D. Marongiu, A. Simbula, V. Demontis, F. Quochi, A. Mura, G. Bongiovanni

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The defect tolerance of hybrid perovskites, which makes their optoelectronic properties minimally affected by defects in their crystal structure or composition, also endows them with ambipolar transport, with both electrons in the conduction band and holes in the valence band equally mobile and responsive to external electric fields. However, ambipolar transport and defect-tolerance hinder directional charge separation, because any electric field created by charge separation is quickly screened by the mobile charges. In presence of ambipolar transport is also very difficult to achieve intentional doping without ruining the perovskite with the non-radiative recombination that comes with deep intragap defect states.

In this work we show an experimental technique based on ultrafast optical spectroscopy that disentangles the dynamics of photoexcited electrons and holes, quantify trapping and non-radiative recombination rates for each of them and measure doping concentration.

The technique is applied to two case studies, where traps and doping are engineered to maximize solar cell performances.

The first one is wide-bandgap thin-film perovskite solar cells with the addition of a controlled amount of two-dimensional transition metal carbides (MXenes Ti_3C_2Cl) to engineer the charge transport. The experimental results, in combination with DFT calculations, provide evidence of photo-doping in devices with MXenes, with charge-selective trapping of holes. These results show that perovskite-MXenes heterojunction can be considered a promising tool to achieve intentional and controlled doping in perovskites optoelectronic devices.

The second case study is methylammonium tin iodide perovskites, both in thin film and single crystal forms. The concentration of background doping is directly accessed by measuring the dynamics of photoluminescence, while transient absorption provides the separate recombination rates for each of the two carrier types. The doping concentration is tracked over the perovskite aging, providing an assessment of the effects of illumination and oxygen/water exposure into the degradation of tin perovskite performances.

STRUCTURAL AND MOLECULAR ENGINEERING OF LOW DIMENSIONAL PEROVSKITES

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Ranita Samanta,[1] **Francesca Canestra**[1]

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Low-dimensional metal halide perovskites are attracting great interest for photovoltaics and photonics. The type of B-site metal in conjunction with the organic templating cations play a crucial role to determine the properties of low dimensional perovskites. Here we discuss how the molecular engineering of organic cations in terms of cationic head (ammonium vs imidazolium – Figure 1, mono- vs di-topic cations) as well as geometry, length and conjugation of the molecular core (alkylammonium and stilbene derivatives) deeply affect the dimensionality, structural and optoelectronic properties of lead and tin perovskites.

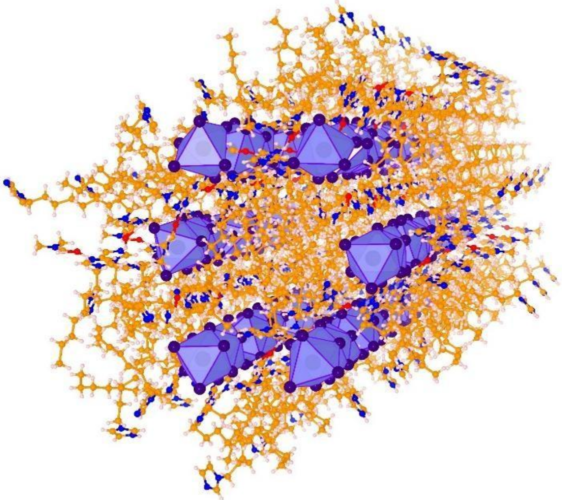

***Figure 1**: Example of low-dimensional ‘perovskitoid’ structure templated by imidazolium cations*

We employ solid state NMR (ssNMR) as a key technique to investigate the local structures at the atomic level via ^{1}H, ^{13}C, ^{15}N, ^{119}Sn and ^{207}Pb ssNMR spectroscopy, providing clear spectral fingerprints which are characteristic of perovskites with different structural motifs, allowing the identification of their supramolecular spatial arrangements.[1] We further apply spin-lattice relaxation dynamics measurements to investigate molecular motions and structural rigidity in low-dimensional systems, and discuss their impact on the perovskites’ luminescence properties, relevant for lasing and photonic applications.[2,3] Our studies shed light on how supramolecular engineering can guide the development of improved materials for optoelectronics.

***Acknowledgements**: European Union’s Horizon Europe Research Council program under Grant Agreement No. 101040681 (ERC Starting Grant SUPER).*

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[3] C. T. Triggs et al, *J. Am. Chem. Soc.* **2025**, 147, 38, 34706–34720.

PEROVSKITES, PHOTOCATALYSIS, CHIRALITY: *CULTIVATING* MATERIALS FROM GROWTH TO FUNCTION

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Compositional design is a central yet often underappreciated driver of materials functionality, extending far beyond simple elemental substitution. In this contribution, we frame materials development as a process of *cultivation*, where deliberate compositional choices during growth encode structure, defects, and interfaces that ultimately determine function. Rather than treating composition as a static parameter, we emphasize its dynamic role in directing structural dimensionality, lattice distortions, and electronic landscapes.

Focusing on perovskite-based materials, we demonstrate how compositional tuning across inorganic frameworks and organic components enables precise control over dimensionality, symmetry, and interfacial chemistry. Such control governs charge localization, transport, and reactivity, allowing functionality to be programmed at the solid-state level. We further show that compositional asymmetry can be exploited to introduce chirality directly into the lattice, generating enantiodifferentiating and spin-selective environments without relying on molecular chiral additives. By integrating compositional design with growth chemistry and structure–property relationships, this work outlines a materials-by-design paradigm in which function is cultivated through rational control of composition across multiple length scales. This approach provides general design principles for adaptive and multifunctional materials, advancing materials chemistry beyond trial-and-error synthesis toward predictive compositional engineering.

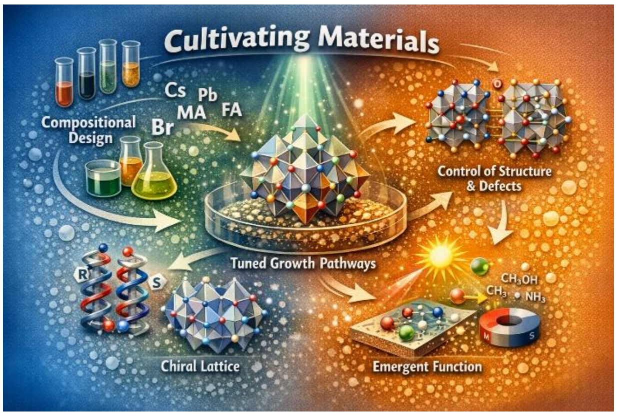

Figure 1: *Pictorial representation of the content of the talk.*

CHALLENGES AND STRATEGIES TOWARDS EFFICIENT TIN-HALIDE PEROVSKITE SOLAR CELLS: A COMPUTATIONAL PERSPECTIVE

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Metal-halide perovskites are outstanding materials for photovoltaics due to their excellent optoelectronic properties, such as the direct and tunable band gaps, the large absorption cross sections and the long lifetimes of the photo-generated charge carriers. Lead-halide perovskites (LHP) dominate the field by showing efficiencies of 26% in solar cell devices, but a valid alternative is represented by tin-halide perovskites (THP), which offer lower band gaps and a more limited toxicity of the metal. Despite the large efforts, the efficiencies of THPs are still sensibly lower than the lead-counterpart, mostly due to the elevated p-doping and the limited stability of tin to oxidation.[1]

Based on a DFT analysis, in this presentation we provide a theoretical account of the main processes limiting the efficiency and the stability of THPs, their defect-related origin and the possible strategies to mitigate the impact of defects.

Through the analysis of the defect chemistry, the origin of the heavy p-doping and the parallel existence of non-radiative recombination channels, as well as the potential defect-activated degradation processes at the surface will be discussed.[2-3] By the study of the electron-phonon coupling, the nature of hole carriers vs doping density is analyzed.[4]

Hence, the discussion moves to illustrate the potential strategies to be adopted to reduce p-doping and improve optoelectronic properties of THPs. The effects of chemical composition (metal and halide alloying) on the p-doping are discussed. In-silico designed de-doping strategies based on the incorporation of trivalent metal ions coupled to small halide-alloying will be presented.[5] Finally, the emerging role of self-assembled monolayers (SAM) as promising hole-selective materials in THPs is discussed by a comparison of their electronic alignment at the interface with the THPs vs LHPs.

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COMPUTATIONAL MODELING OF NEW GENERATION MATERIALS FOR PHOTOVOLTAICS AND PHOTOCATALYSIS

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Hybrid AMX_3 perovskites (A=Cs, CH_3NH_3; M=Sn, Pb; X=halide) have in the last years revolutionized the scenario of photovoltaic technologies. Despite the extremely fast progress, the materials electronic properties which are key to the performance are relatively little understood. We developed an effective GW method incorporating spin-orbit coupling[1] which allows us to accurately model the electronic, optical and transport properties of halide perovskites, opening the way to new materials design. In parallel, a series of different strategies will be reported to increase the device stability and efficiency.[2] While instability in aqueous environment has long impeded employment of metal halide perovskites for heterogeneous photocatalysis, recent reports have shown that some particular tin halide perovskites (THPs) can be water-stable and active in photocatalytic hydrogen production. To unravel the mechanistic details underlying the photocatalytic activity of THPs, we compare the reactivity of the water-stable and active $DMASnBr_3$ (DMA = dimethylammonium) perovskite against prototypical $MASnI_3$ and $MASnBr_3$ compounds (MA = methylammonium), employing advanced electronic–structure calculations. We find that the binding energy of electron polarons at the surface of THPs, driven by the conduction band energetics, is cardinal for photocatalytic hydrogen reduction.[3] In this framework, the interplay between the A-site cation and halogen is found to play a key role in defining the photoreactivity of the material by tuning the perovskite electronic energy levels. Our study, by elucidating the key steps of the reaction, may assist the development of more stable and efficient materials for photocatalytic hydrogen reduction. We report a report is made on a composite system including a double perovskite, $Cs_2AgBiCl_6$/g-C_3N_4, used in parallel for solar-driven hydrogen generation and nitrogen reduction, quantified by a rigorous analytical approach.[4] Finally, a new approach for enantioselective synthesis has been reported with chiral perovskite catalyst. The overall picture of our theoretical investigations underlines a crucial role of computational investigation, casting the possibility of performing predictive modeling simulations, in which the properties of a given system are simulated even before the materials laboratory synthesis and characterization. At the same time, computer simulations are shown to offer the required atomistic insight into hitherto inaccessible experimental observables.

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MECHANISTIC INSIGHTS INTO DIELS-ALDER STEREOSELECTIVITY ON CHIRAL PEROVSKITES

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Although perovskites are predominantly investigated for their outstanding photoelectronic properties, their potential in catalysis has also been recognized,[1] spanning from non-chiral catalytic systems to emerging examples of selective reactions on chiral surfaces.[2]

In this contribution, we present a theoretical study aimed at elucidating the mechanism of a stereoselective Diels-Alder reaction occurring on a chiral perovskite surface. Experimentally, opposite enantioselectivity is observed when switching the chirality of the perovskite catalyst.

To rationalize these observations, we employed a computational protocol integrating solid-state simulations[3] with molecular-level electronic structure calculations.[4] This approach provides us with complementary molecular calculations which help validate the transition-state structures estimated from the solid-state simulations. By comparing reaction pathways in the presence and absence of the perovskite, the simulations reveal how the chiral environment modifies the reaction landscape, selectively stabilizing specific pathways and leading to specific stereochemical outcomes depending on the catalyst chirality.

This work highlights the potential of chiral perovskites as stereoselective catalysts and illustrates how theoretical modeling can provide valuable insights into reaction mechanisms, surface-induced selectivity, and structure-reactivity relationships, ultimately supporting the rational design of novel catalytic materials.

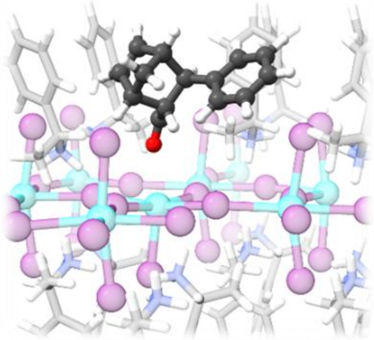

Figure 1: *Representative view of the chiral perovskite surface with one of the possible Diels–Alder products adsorbed.*

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THE OCTAHEDRAL TILTING:
STUDYING THE EFFECT ON TIN HALIDE PEROVSKITES

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Tin Halide Perovskites are promising materials for photovoltaic applications. However, they have received less attention compared to Lead-based Perovskite. Starting from a study on the effect of A-site cation[1] we would understand better the correlation between the structure and the properties of Tin Iodide Perovskite. With this work we analyze the effect of the variation of the dihedral angle (I-Sn-Sn-I) across the z axis, this is equivalent to imagine the tilting of two overlapping octahedra (***Figure 1***).

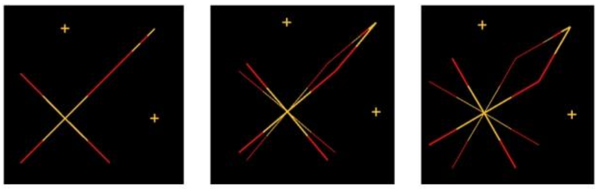

Figure 1*: Top view of two octahedra with dihedral angle increasing from left to right.*

Past works on Lead Iodide Perovskite[2] shows that the geometry structure is determined by the inorganic backbone (lead and iodine) and the octahedra are stable with a dihedral angle of 30° with no strong differences changing the A-Site cation from Cs to methylammonium.

The situation for Tin Iodide, because the favorite geometry for Cs is the cubic one, without tilting or distortion and the dihedral angle is 0°. But when we change the cation for Cs to methylammonium the equilibrium change, and the inorganic backbone prefers to be distorted with a dihedral angle of 25° (***Figure 2***).

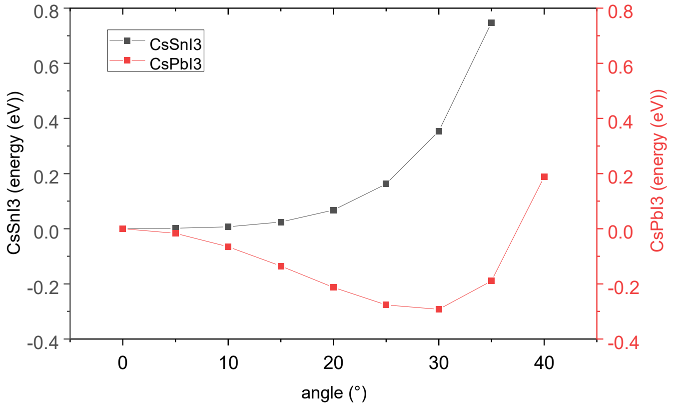

Figure 2*: Energy in function of dihedral angle, black for $CsSnI_3$, red for $CsPbI_3$.*

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GENERATING MOLECULES WITH ARTIFICIAL INTELLIGENCE WITHOUT DATABASES

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One of the central challenges in chemistry is the design of molecules with tailored properties, the so-called molecular inverse design (ID) problem. Addressing this challenge has profound implications across catalysis, drug discovery and, of course, energy harvesting.[1,2] Traditional datadriven machine learning approaches have shown promise in exploring chemical spaces (CSs), but remain fundamentally limited by the need for large, high-quality datasets and costly pre-training procedures.[3,4] In this talk, I will present a novel data-free framework for molecular ID (see Figure 1) that integrates deep reinforcement learning (RL) with quantum chemistry (QC) calculations, enabling the on-the-fly generation and evaluation of molecules without any reliance on pre-existing datasets.[5] As a proof of concept, we applied this approach to toy models targeting ground- and excited-state molecular properties. Our RL-QC engine efficiently explores large CSs using firstprinciples chemical rewards, converging rapidly to optimal candidates and solving the ID problem within known CSs. This promising strategy represents a conceptual shift toward quantum-driven AI for molecular discovery.

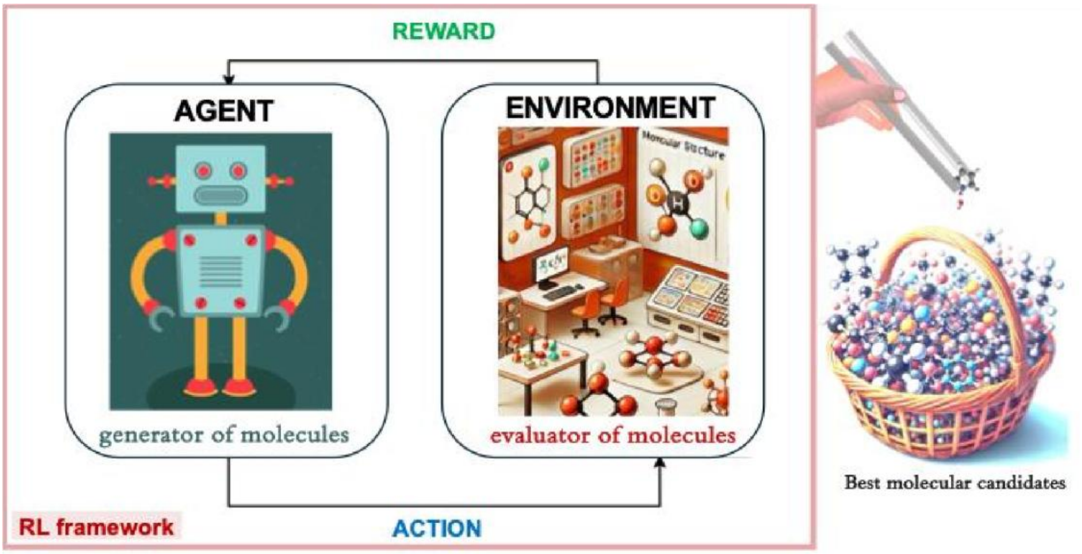

***Figure 1**: Reinforcement learning framework for molecular inverse design.*

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INTERFACE ENGINEERING VIA SELF-ASSEMBLED MONOLAYERS (SAMS) FOR HIGH-EFFICIENCY TIN-BASED PEROVSKITE SOLAR CELLS

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Tin-based perovskite solar cells (PSCs) offer a critical, lead-free alternative for sustainable photovoltaics. Yet, they are hampered by rapid tin oxidation and significant energy losses at charge-transport interfaces. In this talk, I will demonstrate the strategic use of Self-Assembled Monolayers (SAMs), such as carbazole-based phosphonic acids, to replace traditional, bulky polymers like PEDOT: PSS. By anchoring these molecules to the substrate, we successfully tuned the interfacial work function via molecular dipole engineering, creating an energetically favourable alignment that minimises the open-circuit voltage deficit. Furthermore, the SAMs provide a chemical scaffold that passivates surface defects and governs the crystallisation kinetics of the Sn-perovskite film, resulting in a denser morphology with reduced p-type background doping. Our results show that SAM-modified devices not only achieve superior power conversion efficiencies but also exhibit enhanced resistance to moisture-induced degradation. This work highlights interfacial molecular design as a primary lever for overcoming the intrinsic stability and efficiency bottlenecks of tin-based perovskites, paving the way for commercially viable, eco-friendly solar technologies.

STATIC AND DYNAMIC DISORDER IN ORGANIC MIXED IONIC-ELECTRONIC CONDUCTORS

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The diffusion of ions and electronic charges (hole/electron) in Organic Mixed Ionic-Electronic conductors (OMIECs) is profoundly affected by disorder effects.[1] The latter encompass *structural*, *energetic* and *thermal* fluctuations, spanning a wide range of spatial and time domains.

In this contribution, I review our recent findings in modelling disorder effects for two orthogonal classes of OMIECs, namely *non-conjugated polymers* and *conjugated small-molecule* systems (Figure a) and b)). For both classes, the bulk structural properties are investigated by deriving a set of order parameters and auto-correlation functions, to provide detailed atomistic insights into both short- and long-range length scales, as well as to disclose the dynamic effects via molecular dynamics (MD) simulations.

For *non-conjugated polymers,* we introduce a novel strategy to evaluate both static and dynamic disorder effects in the description of the coupled electronic and ionic transport mechanisms.[2] For *conjugated small-molecule systems*,[3] we simulate realistic operational environments, namely the introduction of water in the crystal structures. Under confinement, water changes its structure and dynamics, displaying new static and dynamic properties with respect to the bulk, ultimately impacting the transport phenomena governing the OMIECs device performance.[4]

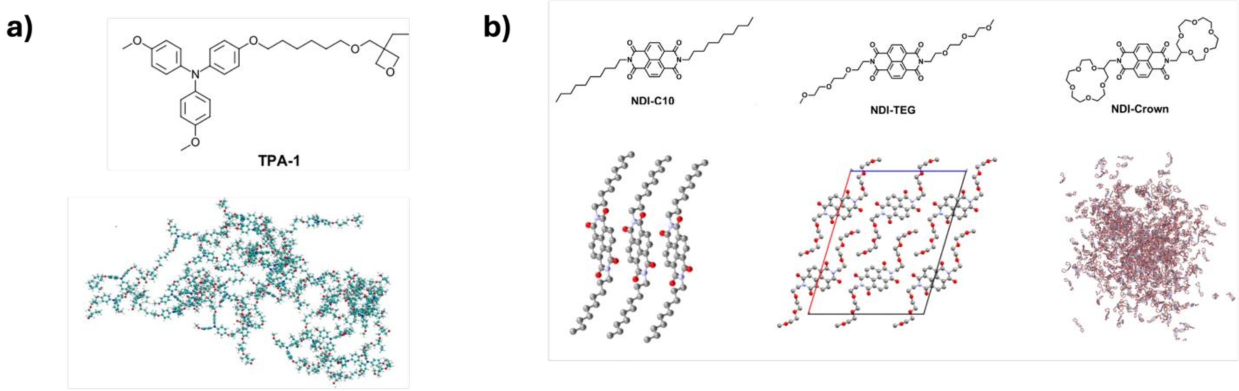

Figure. *Example of OMIECs investigated in this work: a) non-conjugated polymers, b) conjugated small-molecules.*

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JUMP INTO SPACE: HOW PEROVSKITE SOLAR CELLS CAN CONTRIBUTE TO THE NEW SPACE ECONOMY

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The space economy is experiencing exponential growth thanks to the commercialization of near-Earth space related to the increase of internet connectivity on Earth, telecommunication, climate monitoring and weather forecasting, and military surveillance. This growth is reflected in the number of satellites that have been launched from ~1,000 in 2010 to ~10,000 as of 2024.[1] As space missions evolve toward longer durations and higher energy demands, the need for lightweight, high-efficiency, and radiation-hard energy solutions becomes critical.

In this context, perovskites solar cells could play a pivotal role thanks to their high efficiency, robustness, and minimum weight and potential cost-effectiveness.

This contribution presents an overview of frontier technologies for solar energy harvesting, specifically geared for space applications, emphasizing innovations beyond traditional III-V triple-junction photovoltaics (PV) focusing in particular on the role that could be covered by perovskite solar cells.

In addition to that, I will report on our studies related to the resilience of flexible perovskite solar cells to neutrons, which unlike protons and electrons are not electrically charged, and therefore do not directly cause ionization effects in an irradiated material, however, they can cause elastic collisions leaving defects in the lattice.[2]

In particular, I will give an overview on the effects of neutron irradiation on the flexible perovskite solar cells focussing on the role of the specifically sinthetized hole transporting layers (P3HT-modified and PTAA-modified polymers) compared to spiro-OMeTAD.[3,4]

Acknowledgements: *This research has received funding from the European Innovation Council (EIC) under grant agreement No 101162377, JUMP INTO SPACE project and from the Italian Space Agency (ASI), ENFORSPACE project*

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MODELLING GROUND AND EXCITED-STATE PROPERTIES OF MECHANO-LUMINOCHROMIC COPPER HALIDE-BASED COORDINATION POLYMERS

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Mechano-luminochromic copper halide-based Hybrid Coordination Polymers (HCPs) represent a promising class of functional materials for stress and impact sensing through optical responses.[1,2] Among these, HCPs featuring a copper iodide-based ladder structure functionalized with 3Bromopyridine (i.e., $[(CuI)_3\text{-BrPy}]_n$) show remarkable mechano-luminochromic behaviour under UV irradiation, shifting the emission from blue to green upon mechanical grinding.[3]

The atomistic origins of such mechano-induced red-shift are still unclear. To address this issue, we performed first-principles calculations at the density functional theory (DFT) and time-dependent (TD-DFT) level, by computing ground and excited-state properties of $[(CuI)_3\text{-BrPy}]_n$ and exploring different exchange-correlation functional, effective core potentials and basis sets.

Our first-principles calculations show a direct correlation between the Cu-Cu/Cu-I distances with respect to low-lying singlet and triplet excited states. Notably, the Cu-Cu distances are crucial coordinates governing the excited state potential energy profiles, leading to a complex photochemical scenario involving intersystem crossing, phosphorescence as well as thermal activated delayed fluorescence (TADF) mechanisms.

By comparing our DFT/TD-DFT calculations with experimental data (e.g., X-Ray Diffraction, Raman, temperature-dependent steady and time-dependent photoluminescence), a mechanism underlying the mechano-luminochromic behaviour of $[(CuI)_3\text{-BrPy}]_n$ has been formulated. When ground, the emission of $[(CuI)_3\text{-BrPy}]_n$ is assigned to a mixed halide-to-ligand/metal-to-ligand charge transfer triplet excited state (^{3}XMLCT), whereas a TADF mechanism is predominant in the pristine material at room temperature.

Our findings provide a robust framework for understanding the mechano-luminochromic behaviour of Cu-I-based HCPs, allowing for a rational design of piezochromic coatings with tailored sensitivity for force and impact sensing applications.

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HUNTING ELUSIVE POLYMORPHS IN ORGANIC SEMICONDUCTORS AND MIXED IONIC ELECTRONIC CONDUCTORS

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Organic semiconductors, in particular the emerging class of mixed ionic-electronic conductors (OMIECs), are promising functional materials for energy-saving and biomimetic applications.[1] They are based on organic p-electron conjugated systems able to transport ionic and electronic charges. Small molecule based conductors (e.g., acenes, oligothiophenes, naphthalenediimides) exhibit a diverse morphological landscape, encompassing crystalline, amorphous and liquid crystal (LC) phases, which affect the device performance. Structural polymorphs can complicate the picture even further, each one showing distinct charge transport properties. Solid-state polymorphic conversion can easily occur under device operating conditions and may be either beneficial or detrimental to performance.[2] Up to now, an in-depth atomistic understanding of the mechanisms governing polymorphic transitions in soft conjugated materials is missing.

To fill this knowledge-gap, we investigated two naphthalenediimide (**NDI**) derivatives, bearing linear alkyl side chains with six (**NDI-C6**) and ten (**NDI-C10**) carbon atoms.[3] **NDI-C6** presents elusive polymorphs near room temperature, whose crystal structures have only been partially determined. **NDI-C10** instead shows a high-temperature polymorph, followed by a pre-melting LC phase. For both phases, resolved crystal structures are not available. We performed extended atomistic molecular dynamics (MD) and found that a careful re-parametrisation of the force field is crucial to accurately reproduce the experimental crystallographic parameters.[4] We identify the driving force of the polymorphic transitions and characterise the phase change in terms of molecular geometry, collective variables and order parameters, as inspired from the physics of LCs and disordered systems.[4] Moreover, for **NDI-C6** we refine the crystal structure of both the room temperature polymorphs and, for **NDI-C10**, we propose the structure of the high temperature polymorph.

These findings contribute to a deeper understanding of polymorphism in soft functional materials, hopefully leading to the introduction of design principles for controlling the crystal structures and phase stability.

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THEORETICAL MODELING OF ULTRAFAST PHASE TRANSITIONS FROM THE FEMTOSECOND TO THE PICOSECOND SCALE

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In this talk, I will introduce a theoretical approach to ultrafast phase transitions that captures both electron/hole and phonon dynamics following laser pumping, on time scales ranging from a few femtoseconds to several picoseconds after irradiation.

At short times, the method relies on solving the Bloch equations coupled to Ehrenfest dynamics. It includes the electric field of the pump explicitly, as well as carrier–carrier, carrier–phonon, and phonon–phonon scattering, treated entirely from first principles.

At longer times before recombination, when carrier–carrier interactions generate a photoexcited quasi-equilibrium electron–hole plasma, the approach is based on a constrained density-functional perturbation theory (cDFPT) scheme that accounts for the presence of holes in the valence band and electrons in the conduction band (two-Fermi-level approach). In this framework, the calculation of forces, phonon dispersion, and electron–phonon coupling becomes possible, as well as molecular dynamics with machine-learning potentials in the presence of an electron–hole plasma.

I will showcase applications of the method to several materials.

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SODIUM-ION STORAGE IN HARD CARBON

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Owing to the low cost and high abundance of sodium, Na-ion batteries (NIB) represent a viable alternative to the currently dominant energy storage technology, Li-ion batteries (LIB). Na, however, does not intercalate into graphite, the material of choice for anodes in LIB. Hard carbon, an amorphous, nano-porous C-based material, represents the most studied and the best performing anode material for NIB. Due to difficulties of investigating this non-crystalline material, the mechanism of Na storage it not yet known. In particular, it is not clear whether Na is stored in between graphene-like domains, at defects or in the nano-pores. In this talk I will present some preliminary results of our ongoing investigations, where we developed a machinelearning interatomic potential (MLIP) trained on DFT energies and forces to describe the process of intercalation and reduction of Na ions in hard carbon. Using grand canonical Monte Carlo and molecular dynamics calculations, we studied the storage process as a function of the applied potential, controlled via the chemical potential of the Na reservoir. We computed the charge/discharge curve, and we identified a sequence of steps leading to the accumulation of Na, which include adsorption at defects, intercalation between graphene-like domains, and formation of Na clusters. Finally, we correlated structural properties to the storage capacity, highlighting the role of the pore volume.

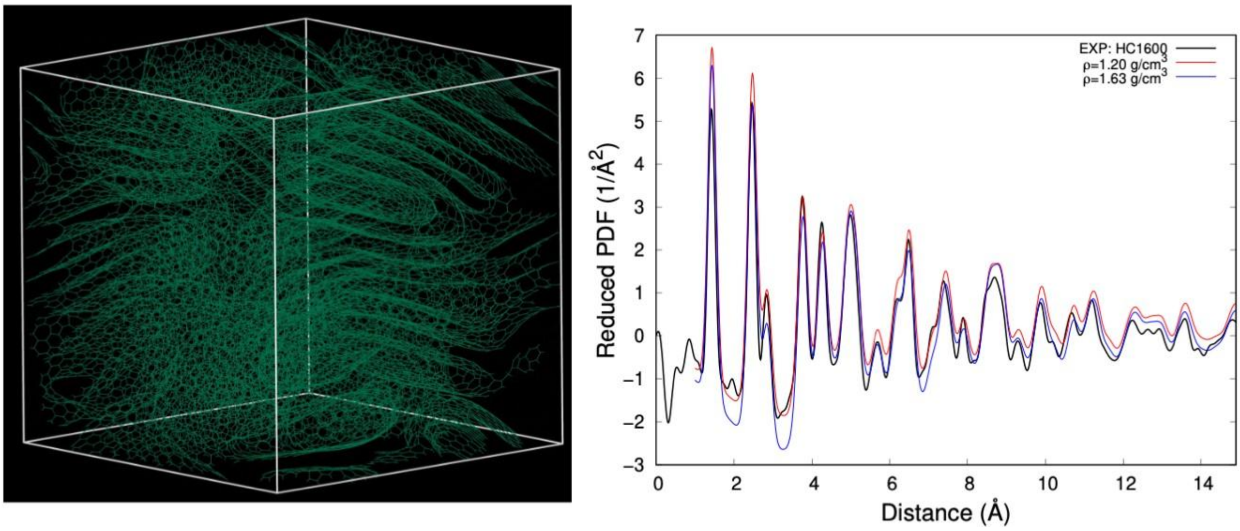

Figure 1: *(Left) Structural model of hard carbon. (Right) Comparison of the reduced pair distribution function against experimental data*

LINKING THE DEGRADATION OF COLORS IN PAINTINGS TO ENERGY APPLICATIONS: CHARGE TRANSFER AND SPIN POPULATION IN PRUSSIAN BLUE

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Several historical colored pigments from paintings of the late 1800s and early 1900s are undergoing irreversible degradation processes, the causes of which remain unclear. Prussian Blue is a mixed-valence compound whose intense blue color originates from intervalence charge transfer between Fe(II) and Fe(III) centers bridged by cyanide ligands.

While this mechanism has long been studied in the context of Cultural Heritage and pigments degradation, the same charge-transfer processes are central to the functionality of Prussian Blue and related materials in modern energy applications, including sodium- and potassium-ion batteries.

In this contribution, we present preliminary results on the electronic structure of Prussian Blue at the atomic scale, focusing on charge localization, intervalence charge transfer, and the associated redistribution of spin populations on iron centers. Optical absorption is also discussed.

The study is carried out by means of a fully theoretical approach based on the density functional theory.

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ADVANCED CHARACTERIZATION AND CO_2 ABSORPTION PROPERTIES OF ZR - AND AL- MOFS BASED ON C_4 LINKERS

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MOFs are crystalline porous solids composed of metal nodes and organic linkers, characterized by exceptionally high surface areas, tunable pore sizes, and adjustable chemical functionalities. These features make them particularly attractive for CO_2 capture, separation, and storage, including post-combustion capture, direct air capture, and selective gas separation processes Zirconium and Aluminum based MOFs have been extensively studied in the recent past for their enhanced stability and easy scalability. The use of C_4 dicarboxylic linkers has been proven to afford new MOFs with ultramicroporous structure and high CO_2 absorption selectivity. The most famous aluminum MOF, which was developed at industrial scale is the Al-fumarate (Al-FUM), sold under the commercial name of Basolite A520 by BASF chemical company. Al-FUM, of formula $Al(OH)(FUM)\cdot 4H_2O$ (FUM^{2-} is the fumarate anion) is isostructural with the terephthalate analogue MIL-53 MOF but having a more rigid structure respect to this latter and smaller pores.[1] Al-fumarate has been employed for many applications ranging from gas storage and separation, pollution remediation, heterogeneous catalysis and as filler for Mixed-Matrix Membranes.[2] In this contribution we report on the syntheses and advanced multitechnique characterization, based on non-ambient X-Ray diffraction, ss-NMR, in situ-FT-IR and DFT calculations, of novel Al- and Zr- MOFs based on C_4 linkers such as aspartic acid, tetrafluoro-succinic acid, mesaconic and itaconic acid. The influence of the functional groups of the C_4 linkers on the CO_2 affinity and its dynamic into the pores will be discussed.

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COMPUTATIONAL METHODS FOR SEMICONDUCTOR TECHNOLOGY

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The development of new methods for energy production and storage in different forms requires the study and design of a new class of materials. Properly engineered materials can improve the efficiency of existing devices or enable the development of entirely new ones.

In this talk, we consider two main case studies. The first concerns the Raman response of highly doped (HD) semiconductors and how this response can be modeled through electron–phonon coupling. Highly doped semiconductors find applications in several optoelectronic devices, such as near-infrared detectors and complementary metal–oxide–semiconductor (CMOS) technologies.

The second case focuses on piezoelectric and ferroelectric materials, which can be exploited in a wide range of technologies based on dielectric materials. A prominent example is hafnium oxide, which has found numerous applications in micro- and nanoelectronics due to its widespread adoption in the semiconductor industry.

This talk will introduce the scientific background of these materials and present computational (in-silico) techniques used to study and design them.

ENERGY DECOMPOSITION–DRIVEN MACHINE LEARNING APPROACHES FOR THE ACCURATE PREDICTION OF REACTION AND ELECTRONIC ENERGIES

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We introduce an interpretable and modular machine-learning framework that improves DFT reaction energies by using physically motivated energy-decomposition descriptors.[1] Linear regression models trained on these components significantly reduce errors with respect to CCSD(T)/CBS references, both through a general model and through reaction-specific models.[2] A random-forest classifier selects the optimal correction model for each reaction, yielding further accuracy gains while preserving interpretability. The approach shows strong robustness in out-of distribution tests on transition-metal systems, outperforming typical neural-network methods in terms of generalization beyond the training set.[3]

Building on this strategy, we developed a functional-independent basis-set extrapolation method that approaches the CBS limit using only double- and triple-ζ DFT calculations.[4] By combining an energy-decomposition scheme with differential-evolution optimization applied to both electronic and relative energies, the method systematically removes the basis-set incompleteness error and elevates low-cost DFT results to chemical accuracy.

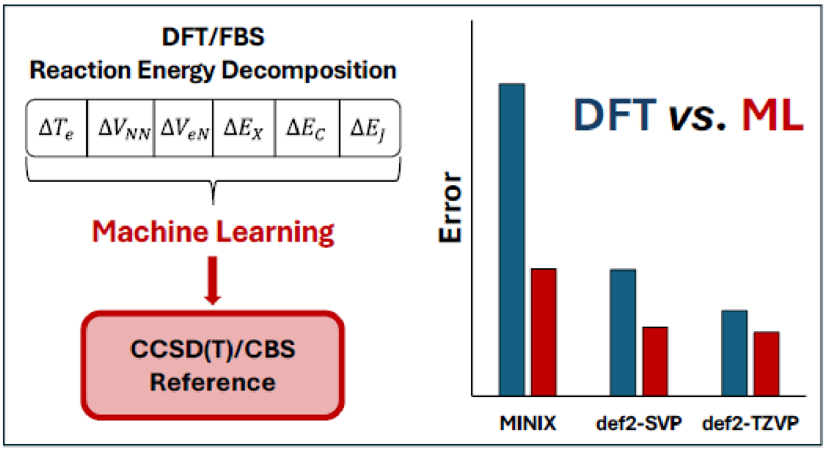

Figure 1: *Coupling Machine Learning with Density Functional Theory to Reduce Basis Set Incompleteness Error and Increase the Accuracy with respect to CCSD(T)/CBS.*

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LEVERAGING MATRIX MODULARITY TO TAILOR THE SPIN STRUCTURE OF MOLECULAR QUBITS

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Molecular qubits offer a highly attractive platform for quantum technologies due to their intrinsic chemical tunability.[1] Among them, pseudo-tetrahedral Cr(IV) complexes have emerged as promising candidates, as they feature well-defined spin states and zero-field splitting (ZFS) parameters that are compatible with optical addressability and coherent spin control.[2]

In this work,[3] we present a computational investigation of Cr(IV) molecular qubits embedded in diamagnetic host matrices, aimed at understanding how the surrounding environment influences their spin properties. By using a multilevel computational protocol that combines periodic calculations with high-level multireference methods, we show that the chemical composition of the host matrix can be used as an effective and independent design lever to modulate the spin structure of the qubit, without altering its molecular structure.

Our results reveal that matrix-induced geometric distortions and electrostatic fields directly reshape the ZFS of molecular qubits. This environment-driven control has direct implications for how molecular qubits store and retain quantum information, as the arrangement of spin sublevels plays a central role in determining their initialization, readout, and robustness to external perturbations.

Overall, this study establishes matrix modularity as a powerful and transferable strategy for engineering the spin properties of molecular qubits, providing predictive insight for the rational design of chemically controlled quantum systems.

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HOMOs/LUMOs ENGINEERING FOR LONG-LIVED EMISSIVE EXCITED STATES IN FE(II) COMPLEXES

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Replacing noble metals with earth-abundant alternatives is a key objective in the development of sustainable photoactive materials for solar energy conversion. Iron, the most abundant metal on Earth, is an attractive candidate;[1] however, Fe(II) polypyridine complexes typically exhibit ultrafast deactivation of metal-to-ligand charge-transfer (MLCT) states due to population of low-lying metal-centered states. Although strong σ-donating N-heterocyclic carbene (NHC) ligands can extend MLCT lifetimes,[2-3] this often results in a narrowed absorption window, limiting solar light absorption. Here, we demonstrate that this trade-off can be overcome by combining strong-field NHC coordination with a HOMO inversion strategy,[4] in which ligand-centered orbitals are raised above the metal-based orbitals, generating a dense manifold of bright, mixed MLCT, ligand-centered, and ligand-to-ligand charge-transfer excited states across the visible region.[5] We report the first Fe(II)–NHC complex incorporating an azaullazine core, which exhibits broad absorption from 350 to 600 nm and an emissive ^{1}MLCT state with a nanosecond lifetime. Crucially, the fused ligand framework defines a LUMO topology that minimizes electronic coupling to low-lying metal-centered states, thereby suppressing nonradiative decay. These results provide the first clear validation of the HOMO inversion concept in iron-based photosensitizers and open new design avenues based on targeted LUMO engineering.

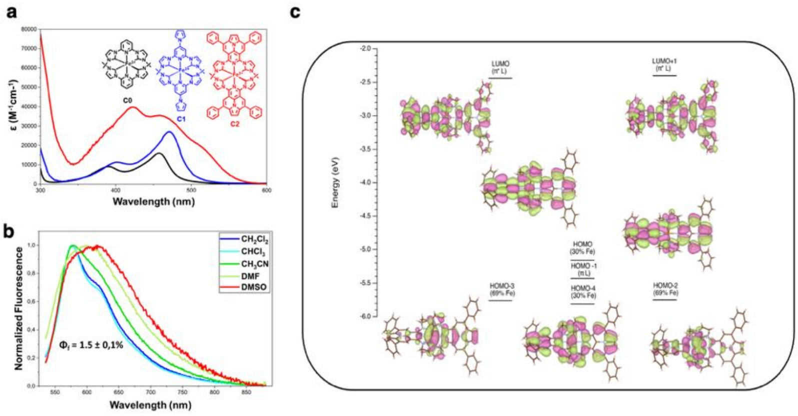

*Fig. 1: : **(a)** UV-VIS absorption spectra of complexes **C0**, **C1** and **C2** in acetonitrile; **(b)** Normalized emission spectra of **C2** Fe(II) complex in solvents of various polarity ($\lambda_{exc.}$ 520 nm); **(c)** Calculated energy levels and isodensity isosurfaces plots of HOMOs and LUMOs of **C2**.*

ADVANCED MODELING OF INTERFACIAL CHARGE TRANSFER AND REACTIVITY IN ENERGY CONVERSION DEVICES

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Understanding charge transfer and reaction mechanisms at materials interfaces at the atomic scale is essential for advancing energy conversion and storage technologies. Yet, these processes often involve electronically complex states that challenge standard density functional theory (DFT).

In this talk, we present recent results from our group illustrating complementary beyond-DFT strategies applied to key energy interfaces. We discuss charge-transfer pathways in molecular photocatalysts anchored on oxide electrodes (DiRh/NiO)[1] and in perovskite solar cells with molecular interlayers,[2] using hybrid DFT and diabatization to quantify interfacial electronic couplings and injection efficiencies. We also address electrocatalytic reactions involving highly correlated intermediates through multireference embedded-cluster and QM/MM approaches, focusing on oxygen evolution in Li-air batteries[3] and IrO_2 catalysts [4] and oxygen activation in bio-inspired dicopper centers.[5] Finally, we show how explicit electric-field simulations enable operando modeling of electrochemical CO_2 activation on defective Bi_2O_3 surfaces under applied bias.

Overall, our results demonstrate how beyond-DFT-based modeling can deliver predictive insights for complex physico-chemical processes at the core of next-generation energy conversion materials and devices.

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SUSTAINABLE MATERIALS AND PROCESSES FOR HALIDE PEROVSKITE PHOTOVOLTAICS

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Halide perovskite solar cells have rapidly emerged as a leading candidate in next-generation photovoltaics due to their high efficiency and cost-effective fabrication. However, their commercial viability remains challenged by environmental and stability concerns. In this work, we present a comprehensive approach to the sustainable development of halide perovskite photovoltaics through environmentally conscious materials and processes. Key strategies include the use of green solvents for perovskite film deposition, enabling safer and more scalable fabrication routes. We demonstrate the fabrication of fully flexible perovskite solar cells under ambient air conditions using low-toxicity, eco-friendly solvents. To further minimize solvent use, we explore solvent-free thermal evaporation as an alternative method for perovskite layer deposition, significantly reducing chemical waste. Additionally, we replace conventional noble metal electrodes with carbon-based back contacts, offering a cost-effective and sustainable alternative with good conductivity and stability, showcasing potential for full roll-to-roll production. Finally, we address the critical issue of lead toxicity by partially substituting lead with tin in mixed Pb-Sn perovskite compositions, achieving reduced environmental impact while maintaining promising photovoltaic properties. Together, these innovations mark significant progress toward greener, safer, and more sustainable perovskite solar technologies suitable for widespread deployment.

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PHOTOCAPACITORS BASED ON EMERGING INDOOR PHOTOVOLTAICS: TOWARD BATTERY-FREE SMART DEVICES

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The synergy between next-generation photovoltaics and integrated energy storage technologies opens unprecedented avenues for powering autonomous electronics, especially under ambient indoor conditions. Photocapacitors[1] - devices that simultaneously harvest and store solar energy - present a promising solution to eliminate battery dependence in Internet of Things (IoT) applications and in portable and wearable electronics.

We report on PSC-based photocapacitors, exhibiting remarkable photocharging voltages under low illumination. The device quickly reaches the saturated voltage under various light intensities and displays a self-discharge of >2 minutes, with overall and storage efficiencies of 2.8% and 23% respectively, with a broad potential window of 3.8 V.[2] We also discuss high-performance three-terminal DSC-based photocapacitors, which combine polyviologen-based asymmetric supercapacitors with eco-friendly fungal membranes. These systems exhibit photocharging voltages up to 920 mV under 1000 lux illumination and achieve photocharging efficiencies up to 18%, with power conversion efficiencies exceeding 30%. Remarkably, such devices outperform commercial amorphous silicon PV modules by a factor of 3.5 in low-light inference throughput, enabling uninterrupted operation of edge-AI IoT systems.[3]

These examples of integrated architectures represent a paradigm shift in self-powered electronics, offering sustainable, battery-free energy solutions that meet the demands of modern digital infrastructure while aligning with global sustainability goals.

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IMPACT OF STRUCTURAL RIGIDITY ON AMPLIFIED SPONTANEOUS EMISSION PROPERTIES OF ALKYLAMMONIUM PEROVSKITES

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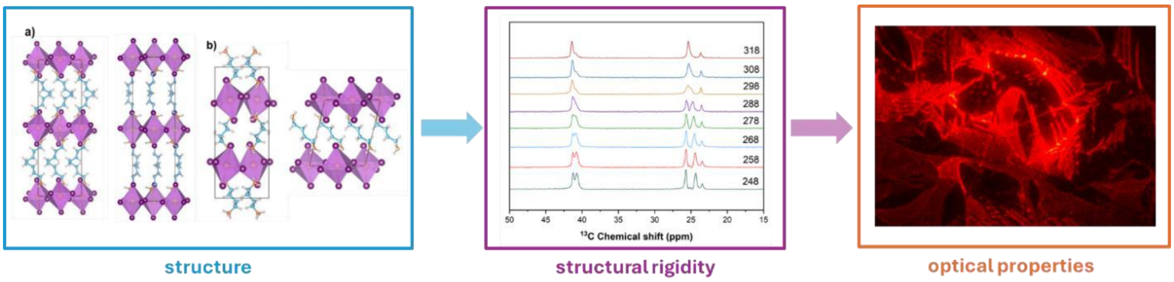

structure

structural rigidity

optical properties

Two-dimensional (2D) tin-based hybrid halide perovskites are emerging as promising lead-free materials for light-emitting and lasing applications, combining strong excitonic effects with reduced environmental impact.[1] In these systems, the nature of the organic spacer cation plays a decisive role in determining lattice rigidity, exciton–phonon interactions, and optical performance. In this work, we present a comparative study of two structurally distinct 2D tin perovskites: the Ruddlesden-Popper phase butylammonium tin iodide (BA_2SnI_4) and the DionJacobson phase 1,4-diaminobutane tin iodide ($DABSnI_4$). Using single crystal X-ray diffraction, Raman spectroscopy, solid-state NMR (ssNMR), and temperature-dependent optical spectroscopy, we establish a direct correlation between structural connectivity, lattice dynamics and optical properties, such as amplified spontaneous emission (ASE). Both materials undergo temperature-driven phase transitions; in BA_2SnI_4 the transition is known[2] and is driven by octahedral rearrangements, leading to a clear change in the photoluminescence (PL). In contrast, $DABSnI_4$ exhibits a phase transition dominated by changes in interlayer spacing, while preserving octahedral tilting, resulting in negligible impact on PL. Analysis of ^{13}C ssNMR relaxation times using the Bloembergen-Purcell-Pound model reveals higher activation energies for cation dynamics in $DABSnI_4$, indicating a more rigid lattice.[3] Temperature-dependent PL[4] linewidth analysis shows weaker exciton-phonon coupling and lower exciton binding energy in the DJ phase. Therefore, ASE is observed exclusively in $DABSnI_4$, with a low threshold of ~25 µJ cm^{-2} at 78 K, making it the first 2D tin-based perovskite to exhibit ASE, while BA_2SnI_4 shows no ASE. These results identify lattice rigidity as a key parameter for coherent emission in 2D tin perovskites and highlight Dion-Jacobson phases as promising candidates for lead-free perovskite lasers.

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AB-INITIO CALCULATIONS OF MASS SPECTRA

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Mass spectrometry (MS) is a central analytical technique for molecular structure elucidation across chemistry, biology, and materials science. Its sensitivity and rich fragmentation information make it indispensable in applications ranging from metabolomics to drug discovery. However, reliable interpretation of tandem mass spectra remains challenging for structurally complex molecules due to multiple competing dissociation pathways, congested fragment patterns, and limited coverage of reference spectral databases, which complicate automated identification and mechanistic understanding.[1,2]

Computational approaches are therefore essential to support spectral interpretation and annotation. Rule-based tools capture known fragmentation motifs but exhibit limited transferability to unseen chemistries.[2] Machine-learning (ML) models, such as CFM-ID and NEIMS, achieve high predictive accuracy on in-domain datasets,[3,4] yet provide limited mechanistic insight and often degrade in performance for chemically diverse or underrepresented compound classes. Quantum chemistry–based methods (QCEIMS, QCxMS, QCxMS2) offer improved physical rigor and mechanistic interpretability and, when combined with efficient xTB Hamiltonians and CREST conformational sampling, have become increasingly practical for larger systems.[5] Nevertheless, the computational cost of these methods increases rapidly with molecular size, and scalability remains constrained by available computational resources, while predictive accuracy for structurally complex systems remains limited.

To address these limitations, we present a unified, ab-initio top-to-bottom computational pipeline for predicting tandem mass spectra from molecular structure and energetics, integrating protomer generation, semi-empirical optimization, and energy-based ranking within a multi-level screening framework. Fragmentation pathways are enumerated using an in-house graph-based algorithm and filtered by energetic feasibility to generate physically consistent simulated MS/MS spectra while controlling combinatorial growth and computational cost.

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INNOVATIVE MATERIALS FOR TANDEM SOLAR CELLS

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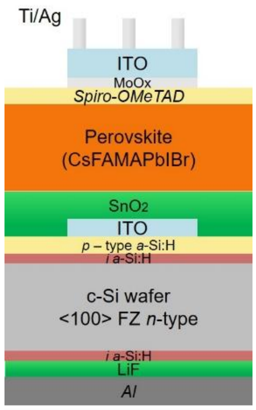
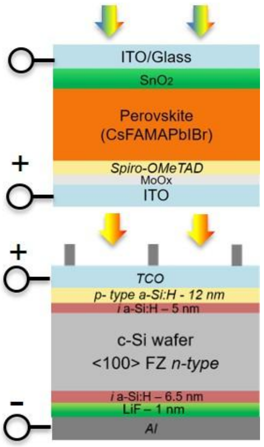
Within the GoPV project, ENEA is focusing on the development of innovative materials for high-efficiency perovskite/silicon tandem solar cells. While silicon heterojunction (SHJ) and perovskite solar cells (PSCs) individually achieve power conversion efficiencies (PCEs) above 27%, their monolithic integration enables broader spectral utilization and has already delivered record efficiencies around 35%. Despite this potential, several challenges must be addressed to enable scalable and cost-effective deployment. The main issues concern the intrinsic instability of hybrid perovskites, the parasitic absorption and processing complexity of doped amorphous silicon contacts, and the reliance on indium-based transparent conductive oxides (TCOs).

ENEA's strategy focuses on three directions: (i) replacing hybrid perovskites with the all-inorganic $CsPbI_3$, expected to offer enhanced thermal and photostability, (ii) developing dopant-free selective contacts (MoO_x, LiF, and self-assembled monolayers (SAMs)) to simplify processing and reduce optical losses, and (iii) reducing or eliminating the use of indium in TCOs.

In parallel, we developed low-temperature device architectures for $CsPbI_3$-based PSCs, investigating both nip and pin configurations. PCEs up to 9% were achieved in nip devices using SnO_2 as electron transport layer, while up to 16% were obtained in pin devices employing 2PACz SAM as hole transport layer. Finally, proof-of-concept tandem devices were demonstrated in both four-terminal and monolithic configurations, employing the device structures illustrated in the figure below.





SYNTHESIS OF INDIUM-OXIDE-BASED TRANSPARENT ELECTRODES AND SnO_X INTERLAYERS FOR TANDEM SOLAR CELLS

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Contribution intended for the GOPV Session - UniCT partner

Photovoltaic (PV) technologies are pivotal for reducing the environmental footprint of power generation; consequently, substantial efforts are currently devoted to improving the power conversion efficiency of predominantly single-junction solar cells. In this context, tandem solar cells have emerged as a key strategy to increase efficiency while reducing land use for PV installations. In perovskite/silicon tandem architectures, approaching the theoretical efficiency potential and reaching competitive device performance critically depends on the transparent electrodes. These elements need to combine high carrier mobility with minimal optical losses, and their production must comply with the cell production flow.[1] Zr-doped indium oxide (IZrO) could be a suitable wide-bandgap front electrode, whereas Zn-doped indium oxide (IZO) makes a good candidate as a middle transparent electrode to mitigate near-infrared losses.[2] Taking all this into account, here we report the synthesis and characterization of RF-sputtered indium-oxide based TCOs, namely IZO and IZrO. When deposited onto semi-finished bare SHJ substrates, both IZO and IZrO induce a measurable decrease in surface photovoltage (SPV) and implied V_{OC}, suggesting sputtering-related degradation of the surface passivation.[3,4] Consistently, EQE/IQE measurements reveal a reduced spectral response after TCO deposition, pointing to interface-limited carrier extraction at the TCO/cell junction. These observations motivate the development of sputtering-compatible interface strategies, including the evaluation of thin SnO_x-based buffer layers to mitigate plasma-induced damage while remaining compatible with perovskite interface in tandem solar cells. In such a context, we are also investigating SnO_2 as an electron-selective transport layer due to its established chemical stability and favorable interface compatibility with perovskite absorbers, providing a relevant material platform for tandem-oriented interfacial engineering.[5]

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DFT INVESTIGATIONS ON THE HALOGEN BOND-DRIVEN REVERSIBLE THERMOCHROMISM IN A 2D HYBRID PEROVSKITE

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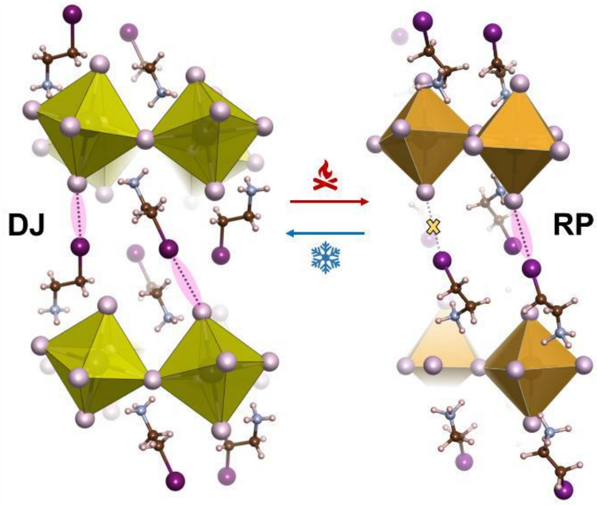
Halogen bonding (XB) is proposed as a supramolecular handle to reversibly trigger a single-crystal phase transition in a 2D metal–halide perovskite using a low-energy thermal stimulus. Using 2-iodoethylammonium ($2IEA^+$) as a "telechelic" tecton that can donate both hydrogen bonds (HB) and halogen bonds, heating modulates XB strength by inducing reversible cation isomerization, which drives a stacking change from Dion–Jacobson-like (DJ) to Ruddlesden–Popper-like (RP). To rationalize this behavior, DFT calculations are performed on isolated $2XEA^+$ cations (X = Cl, Br, I) in both syn and anti conformations to compare structural features, thermodynamic stability, and electronic descriptors—especially the maximum molecular surface electrostatic potential used to estimate the halogen "σ-hole". Periodic DFT is also used on (2IEA)2PbI4 to compute band gap, density of states, and charge-carrier effective masses, then relate these quantities to experimental observations, alongside a noncovalent-interaction analysis focused on characterizing XB in the solid.



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SUBSTITUTIONAL N-TYPE ELECTRONIC DOPING OF LEAD-HALIDE PEROVSKITES

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Despite being central to conventional semiconductor technologies, intentional electronic doping remains challenging in metal halide perovskites; however, even subtle doping can directly modulate their electronic properties and mitigate interfacial energy-level misalignment, exerting a disproportionate influence on device performance without introducing transport barriers. In this work, we demonstrate controllable electronic doping by introducing Ytterbium (III) chloride ($YbCl_3$) as an intentional n-type dopant into lead halide perovskites. Combining density functional theory (DFT) calculations, Kelvin probe measurements, and solid-state NMR spectroscopy, we demonstrate that trivalent Yb^{3+} induces effective n-type doping in perovskites, evidenced by a continuous up-shift of the Fermi level across the bandgap and direct atomic-scale confirmation of Yb lattice incorporation. When applied in inverted perovskite solar cells (IPSCs), the gradient n-doping profile across the perovskite thin films promotes the efficient hole extraction across the perovskite/hole-transport-layer interface and suppresses nonradiative recombination at the perovskite/C_{60} interface, as corroborated by transient spectroscopic analyses and numerical simulations. Accordingly, the mixed-halide IPSCs with a large bandgap of 1.84 eV achieve a remarkable PCE of 19.51%, setting a new benchmark among counterparts with bandgaps exceeding 1.80 eV. The versatility of trivalent doping was also proved by the boosted performance of inverted PSCs with bandgaps of 1.77 eV and 1.55 eV, yielding a PCE of 20.28% and 26.08%, respectively. This work highlights the strong applicability of electronic doping for both single junction and tandem photovoltaics and can be extended to other electronic devices.

LOW-DIMENSIONAL HYBRID PEROVSKITES FOR WIDE-BANDGAP PHOTOVOLTAIC APPLICATIONS

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Low-dimensional hybrid perovskites (LD-HPs) are gaining increasing attention as wide-bandgap absorbers for stable and versatile photovoltaic technologies, particularly within tandem architectures where materials with tuneable band gap are required. Their layered structure, defined by bulky organic spacer cations separating n inorganic octahedral slabs, enhances environmental stability but introduces pronounced anisotropy in charge transport.[1] As a result, controlling both growth orientation and phase composition is essential to unlock their full potential.

In low-n systems, LD-HPs can be readily obtained as phase-pure materials, yet their efficient operation is strongly limited by inefficient out-of-plane transport unless a preferential vertical orientation of the inorganic layers is achieved.[2-3] As the targeted bandgap is reduced toward values relevant for tandem and indoor photovoltaic applications, higher-order phases (n = 3 and n = 4) become increasingly relevant. In this regime, vertical orientation is no longer the primary limiting factor, while maintaining phase purity emerges as the dominant challenge, with mixed-phase formation severely impacting the resulting optoelectronic properties.[4] The presence of mixed phases leads to spatial variations in optoelectronic properties across the film, severely limiting device performance. These distinct regimes highlight the need for n-dependent materials design strategies.

Here, efficient LD-HP devices are presented, employing n = 2, n = 3, and higher-n phases for colour-tuneable applications, achieving power conversion efficiencies of up to 10%. Crucially, we identify materials-level design principles to control crystal orientation and phase purity in LD-HPs, supporting their development as wide-bandgap materials for tandem photovoltaic applications and device-integration strategies. Beyond their use as absorbers, LD-HPs are also employed as surface passivation layers to enhance the performance of three-dimensional-based perovskite solar cells.[5]

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OPTIMIZATION OF 4-TERMINAL ALL-PEROVSKITE TANDEM SOLAR CELLS: EXPERIMENTS AND OPTO-ELECTRICAL SIMULATIONS

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The enhanced light absorbance of mixed Pb–Sn perovskites up to a wavelength of 1000 nm and their new record PCEs for single-junction cells (up to 24%) make them promising for application in all-perovskite tandem solar cells to exceed current efficiency limits. However, the rapid oxidation of Sn^{2+} cations during the fabrication process and solar cell operation, as well as the fast crystallization of films, negatively affect the open-circuit voltage (V_{OC}) and the fill factor (FF). At the same time, non-radiative recombination at the surface and grain boundaries of wide-bandgap lead perovskites used for the top subcell also limits the photovoltaic parameters of devices.

In this work, high-efficiency four-terminal (4T) perovskite-based tandem solar cells were developed by combining wide-bandgap perovskites (1.6–1.92 eV) for the top cell with a Pb–Sn perovskite-based bottom subcell (1.26 eV).

For the fabrication of wide-bandgap perovskites used for the top subcells, a hybrid process based on vacuum co-evaporation of halide salts followed by spin-coating of organic salts was optimized to obtain absorbers with bandgaps of 1.6 and 1.75 eV. In addition, a fully inorganic $CsPbI_2Br$ absorber with a bandgap of 1.9 eV was fabricated exclusively by co-evaporation. The influence of different hole transport layers (HTLs) and interfacial passivation on the optoelectronic and electrical properties of the devices was investigated.

The photostability of devices with perovskites obtained by the hybrid method was tested under operating MPPT conditions at 45 °C. In particular, the p–i–n configuration with the HTLs NiO_x/Me-4PACz maintained a high PCE for more than 700 h of continuous illumination.

For the fabrication of the narrow-bandgap perovskite $APb_{0.5}Sn_{0.5}I_3$ (A = Cs, MA, FA) used for the bottom subcell, various additives (SnF_2, 4F-PEAI, GASCN, KSCN, $Pb(SCN)_2$, and Gly·HCl) were employed, and their influence on the morphology, photoluminescence, and photovoltaic properties of mixed Pb–Sn perovskites was studied comparatively. Alternative hole transport layers (PTAA/PFNBr and NiO_x) were also explored as potential substitutes for PEDOT:PSS in the bottom p–i–n subcell. The optimal combination of additives, passivation, and transport layers allowed PCEs of 18.6% for the Pb–Sn bottom cells and 23.6% for the four-terminal solar cells to be achieved. Complementary opto-electrical simulations showed that optimized architectures (featuring thinner ITO, improved optical coupling layers, and reduced non-radiative losses) can raise the efficiencies of all-perovskite 4T tandems realized in this configuration to about 26%, with a projected potential close to 30%, outlining a clear pathway toward next-generation devices with high efficiency and stability.

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INTERFACE AND DEFECT ENGINEERING IN METAL-HALIDE PEROVSKITES: FROM MOLECULAR DESIGN TO IONIC EFFECTS

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Understanding and controlling electronic properties at molecular, interfacial, and ionic levels is essential for advancing metal-halide perovskite solar cells. Here, density functional theory is employed to elucidate how targeted chemical modifications influence charge transport and interfacial energetics across key device components. Heteroatom substitution (O, S, Se) in spiro-like hole-transport materials is shown to induce controlled deviations from planarity and dipole asymmetry, which govern aggregation behavior and modulate hopping-mediated hole mobility. Extending this molecular design strategy to interfaces, a sulfur-functionalized self-assembled monolayer for wide-bandgap perovskites exhibits enhanced binding and electronic coupling at both NiO_x and perovskite surfaces, supported by cooperative π-π stacking and favorable energy alignment. Together, these results highlight how rational molecular engineering and ionic control can be leveraged to tailor interfaces and electronic structure in high-performance perovskite solar cells.

ENGINEERING PEROVSKITE SOLAR CELLS WITH TWO-DIMENSIONAL MATERIALS

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Liquid-phase exfoliated (LPE) two-dimensional materials offer a scalable and industry-compatible route for integrating advanced functionalities into perovskite solar cells (PSCs). We aim to present an overview of the advances enabled by LPE 2D materials produced by BeDimensional, including transition metal dichalcogenides and monochalcogenides (e.g. MoS_2, WS_2, SnS), few-layer graphene (FLG), and few-layer hexagonal boron nitride (*h*-BN).[1] LPE MoS_2 and related materials were used as passivating and buffer interlayers in both hole- and electron-transport layers, in which they improved interfacial energetics, suppressed non-radiative recombination, and enhanced operational stability. Few-layer graphene was introduced as a conductive additive in electron-transport layers to boost charge extraction and as a filler in carbon pastes for carbon-based PSCs, enabling low-cost and scalable architectures.[2,3] Finally, LPE *h*-BN was incorporated into polymer encapsulant layers to improve barrier properties and thermal management, contributing to long-term device stability and environmental safety. Overall, this work demonstrates how industrially produced LPE 2D materials can be deployed across the entire PSC stack, bridging high device performance with manufacturability and durability.

Acknowledgements: *This project received funding from the European Union's LAPERITIVO Horizon Europe innovation action under grant agreement No. 101147311 and 2D-PRINTABLE Horizon Europe research and innovation program under Grant Agreement No. 694101 This project received funding from the Italian Ministero della Transizione Ecologica (MITE), GO-PV project.*

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MOLECULAR DYNAMICS–DRIVEN MODELING OF CARBON NANOMATERIALS FOR ENERGY ABSORPTION

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Carbon-based nanomaterials represent a key class of materials for energy-related applications, particularly in CO_2 capture, gas separation, and energy storage, due to their tunable porosity and favorable adsorption properties. A molecular-level understanding of gas–surface interactions is therefore crucial to optimize their performance under realistic operating conditions. In this contribution, we present a computational framework combining classical molecular dynamics simulations with semiempirical interaction models to investigate gas adsorption phenomena on graphene-derived and graphyne-like nanomaterials.

Accurate force fields based on the Improved Lennard-Jones (ILJ) formalism are developed and validated against high-level *ab initio* reference data, following and extending recent studies on greenhouse gas adsorption on carbon nanomaterials.[1] The methodology is applied to mono- and multilayer carbon nanostructures, including graphtriyne-based membranes, to analyze CO_2 adsorption energetics, selectivity with respect to N_2 and H_2O, and the role of pore architecture and stacking effects, in line with recent molecular dynamics and DFT investigations.[2] The results provide detailed insights into the mechanisms governing CO_2 confinement and storage at the nanoscale, highlighting key structure–property relationships relevant for carbon-neutral energy technologies. Overall, this work demonstrates how atomistic simulations can effectively support the rational design of carbon-based materials for CO_2 capture and energy storage applications.

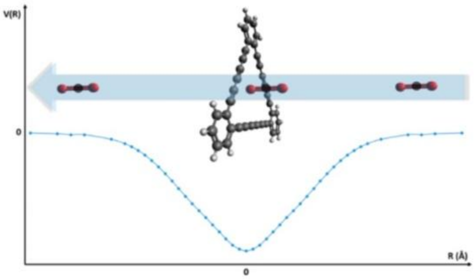

***Figure 1**: Representation of the γ-Graphynes for selective CO_2 capture*

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NON-INVASIVE TRANSDUCTION OF ACTION POTENTIALS WITH PRINTED POLYMER TRANSISTORS

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Action Potentials (APs) of excitable cells contain crucial information about cells physiology. Most of electrical tools available to probe APs are either invasive or require complex manufacturing processes. Minimally invasive and high-throughput recording of intracellular APs in electrogenic cells with scalable technologies is in high demand. Here, focusing on cardiomyocytes monolayers, I will illustrate a powerful and unprecedented approach to combine high-fidelity transduction of APs, typical of gold-standard patch clamp, and scalability of the electrophysiology tool, typical of micro-electrode arrays, exploiting Electrolyte Gated Field-Effect Transistors (EGFETs) based on ink-jet printed polymer semiconductors.[1] Remarkably, despite the planar geometry of the device, we could demonstrate the spontaneous recording of AP waveforms, without recurring to external stimuli, like electro- or opto-poration. The simplicity of the device combined with the high signal to noise ratio opens up new opportunities for low-cost, reliable, and flexible arrays for high quality parallel recording of cellular APs.

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DECIPHERING PHASE STABILITY AND SOLID-STATE TRANSITION PATHWAYS IN P2-LAYERED OXIDES FOR NA-ION BATTERIES

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Layered Transition Metal Oxides (Na_xTMO_2) are the most promising high-energy cathode materials for Na-ion batteries thanks to their convenient anion redox activity.[1] Their structure consists of TMO_2-octahedra 2D slabs sandwiched between Na layers, wherein the arrangement and packing of oxide layers define distinct material morphologies such as P2- and O3- structures.[2] While mixed transition metal oxides in this class of cathodes have shown very good electrochemical performances their long-term stability remains a challenge.[3] This instability is often attributed to solid-state phase transitions during Na^+ insertion and extraction cycles, leading to structural collapse and significant capacity loss. Understanding and controlling these structural transformations is therefore of outmost importance to improve the electrochemical performance of layered oxides.[4] Employing the variable cell nudged elastic band (VC-NEB) method combined with state-of-the-art density functional theory (DFT) calculations,[5,6] we address the prototypical case of P2 ↔ P2'/OP4 transitions in Na_xMnO_2 material and its Ni-doped variant. We reveal the key P2-to-OP4/O2 and P2-to-P2′ transitions that occur across various sodiation levels, involving substantial rearrangements around the transition metal sites, with tetrahedral transition states accountable for energy barriers.
Our analysis of bond length and angle distortions highlights that shear deformations are pivotal in triggering P-to-O gliding at low sodium levels. Based on these insights, our structural distortion metrics offer a straightforward and computationally efficient descriptor to evaluate structural integrity for these layered oxides, enabling the design of NIBs with improved stability and extended lifespan.

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PROBING LIQUID INTERFACES: FROM AIR/WATER TO SOLID/LIQUID SYSTEMS VIA SFG AND MOLECULAR DYNAMICS

D. Lesnicki

Understanding the molecular level structure and dynamics at aqueous interfaces is central to many processes in physical chemistry, ranging from atmospheric chemistry to surface catalysis. In this contribution, we present a comprehensive investigation of molecular orientation, acid-base behavior, and interfacial water structure using a combination of phase-sensitive sum frequency generation (SFG) spectroscopy and first-principles molecular dynamics simulations. Our most recent study[1] explores the pH dependent orientation of pyruvic acid at the air/water interface, revealing distinct tilt angles of protonated and deprotonated functional groups and pH induced reorganization of the interfacial hydrogen-bonding network. These findings demonstrate how interfacial deprotonation equilibria and water dipole orientations couple at molecular scales, offering deep insights into surface acid-base chemistry relevant for environmental and electrochemical interfaces.

We contextualize these results within our previous collaborations, where complementary SFG techniques and density functional theory-based molecular dynamics were used to characterize interfacial behavior of organic acids and solvents. This body of work demonstrates how combining advanced nonlinear vibrational spectroscopy with atomistic simulations can unravel structure-dynamics relationships at complex liquid interfaces, enabling interpretation and prediction of interfacial phenomena with molecular specificity.

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TOWARDS DEVELOPING A SWISS ARMY KNIFE FOR NON-COVALENT INTERACTION

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Despite the growing importance of non-covalent interactions in modern chemistry, the range of computational tools available for their visual analysis remains limited. For this reason, over the past two years we started working in the development of a toolkit able to identify and quantify the strongly dispersion-interacting regions in a molecular system. The toolkit currently enables the computation of a molecular dispersion potential (MDP), which maps key interaction sites by scanning molecular surfaces with a probe atom (e.g., He), and the application of the Atomic Decomposition of London Dispersion (ADLD)[1-2] method that dissect the interaction between molecular fragments to determine London Dispersion contributions of individual atoms and functional groups with a *gold standard* accuracy. We expect that this tool will find applications in molecular design and in asymmetric catalysis. Notably, ADLD has already been adopted and applied by different research groups in the context of asymmetric catalysis.[3-6]

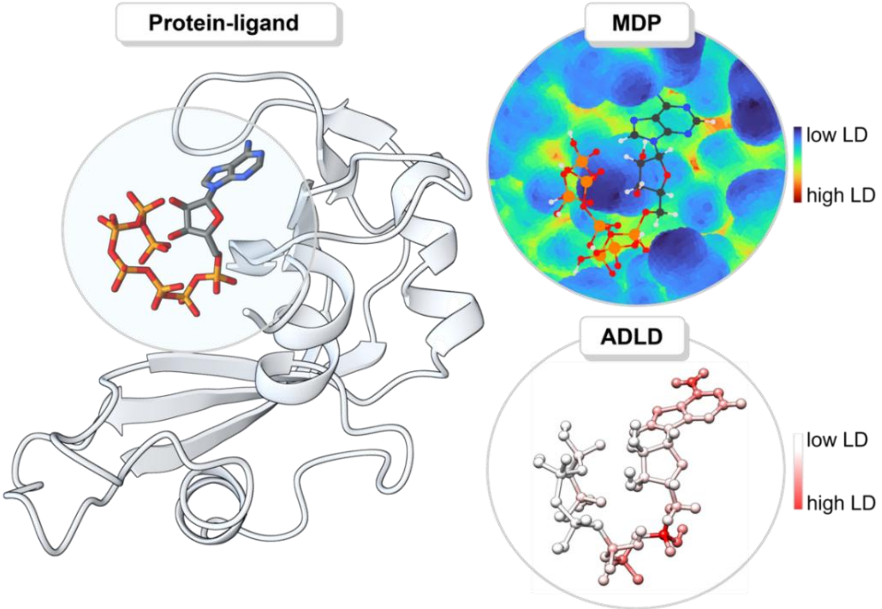

Figure 1: *Dispersion analysis of protein–ligand interactions. The protein–ligand complex is shown on the left. The Molecular Dispersion Potential (MDP, top right) highlights regions of high dispersion interaction on the protein surface, while the Atomic Decomposition of London Dispersion (ADLD, bottom right) identifies the functional groups of the ligand that contribute most to the dispersion interaction.*

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MAGNETIC POLARITONS: SPINS EMBEDDED IN MICROWAVE PLANAR RESONATORS

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Spin is the prototypical two level system, yet its interaction with electromagnetic field is extremely low. By selecting suitable spin systems and designing dedicated resonators, it is possible to enhance the coupling between electronic spins and microwave cavities and drive this hybrid system through different coupling regimes. I shall briefly review possible strategies to fine tune the different parameters and how we obtained strong coupling with molecular spin ensembles[1] and ultra-strong coupling regime with magnons[2,3] coupled to planar superconductor resonators.[4] In the former case, the strong coupling allows us to perform coherent manipulation of molecular spins.[5,6,7] In second case, we explore non linear effects in hybrid magnonic- superconductor bilayer.[9] Finally I shall present a case in which the ultra fine control of the dissipation of molecular spins in microwave cavity allows us to control perfect absorption at few photon regime.[8]

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CONTROLLING LIGHT-MOLECULE INTERACTIONS THROUGH NANOPLASMONICS: INSIGHTS FROM MULTISCALE MODELS

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Localized Surface Plasmons (LSP) are collective excitations of conduction electrons in nanostructures. They became a versatile tool to manipulate light and electromagnetic interactions at the nanoscale. In particular, when molecules are in close proximity of plasmonic nanostructures, the molecule-light interaction is mediated by the plasmonic excitation and a plethora of new phenomena may develop, from surface enhanced spectroscopies (e.g., Surface Enhanced Raman Scattering, SERS), to photoprotection by rapid molecular excitation quenching. In this talk I will focus on two specific phenomena, that are attracting interest also in terms of possible chemical storage of light energy. The first is the situation where the interaction between molecular excitations and the LSPs is so strong to give rise to hybrid states (called plexcitons) that can modify the photophysics and the photochemistry of the molecule.[1] The second is related to the excited ("hot") electrons and holes that are left in the nanostructure after the LSP has dephased, that can be injected into a nearby molecule starting a reaction.[2] For both such phenomena, I will describe the specific multiscale modeling approach we have developed and present relevant examples.[3-6]

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POLARITONIC BLOCH THEORY IN MULTIMODE QUANTUM CAVITIES

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Cavity quantum electrodynamics provides a powerful platform to manipulate material properties, yet its influence on the fundamental structure of crystalline states has remained largely unexplored.[1] Here, the Bloch theorem is extended to crystals in the regime of strong light– matter coupling, demonstrating that polaritonic eigenstates retain a Bloch-like form and that quasimomentum remains a well-defined conserved quantity. By explicitly characterizing the structure of these polaritonic Bloch functions, a clear picture emerges of how electronic and photonic degrees of freedom combine within the lattice.

The role of multimode cavity fields is then considered. The results indicate that additional modes contribute to the system's energy, although their effect on the polaritonic states is subleading compared to the dominant resonant mode, becoming relevant primarily at low frequencies[2] (Figure 1). Moreover, in the single-photon regime, multimode effects reduce to an effective field that is spatially uniform across the crystal plane.

These findings not only formalize the single-mode and long-wavelength approximations for extended crystals but also clarify the conditions under which multimode effects become significant,[3] providing a solid foundation for the theoretical description and design of polaritonic phenomena in crystalline solids.

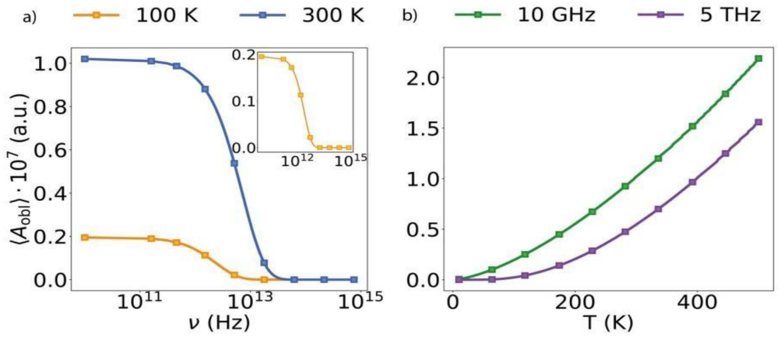

Figure 1: *Expectation value of the multimode field at different temperatures (a) and cavity frequencies (b).*

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RELATIVISTIC POLARITONIC CHEMISTRY : A WAVE-FUNCTION BASED AB INITIO PERSPECTIVE

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The use of quantum light is revolutionizing the concept of chemical manipulation of matter. Strong coupling to light can in fact modify the electronic and the magnetic properties of molecules.[1]
Recently, the group of Prof. Affronte in Modena designed new experiments based on superconducting cavities, coupling electronic spins of single-molecule-magnets with the magnetic component of a quantum field.[2] This opens doors for several technological applications (e.g. quantum computing).
Despite very attractive, the fundamental physics underlying these phenomena is still unclear.
Theoretically, much progress has been done in the field to try answering these questions. In fact, several *ab initio* quantum chemistry methods (DFT, CC, CI, etc.) have been extended to investigate molecular systems in strong light-matter coupling conditions.[3,4]
In this seminar, we will present a new Relativistic Hartree-Fock theory for coupled electronphoton systems.[5] Indeed, the inclusion of relativistic effects becomes crucial if heavy elements are present in the system and more generally if magnetic properties needs to be investigated. This is exactly the context of the experiments performed by Affronte's group. During the talk, the proposed methodology will be explained and its application to small molecular systems containing heavy atom will be presented. Particular attention will be devoted to the analysis of the competition between relativistic and field induced effects.

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COLLECTIVE EFFECTS IN POLARITONIC CHEMISTRY

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Polaritonic chemistry recently emerged as a new way to non-invasively control and manipulate the properties of molecules and materials by exploiting the strong coupling between light and matter.[1] This can be achieved by placing molecules in optical devices such as Fabry-Pérot cavities, generating mixed states with partial light and matter character known as "polaritons".[2]

Recent experiments have demonstrated that optical cavities could be used as an effective tool to control chemical reactivity.[3] However, the physics behind many of these processes remains unclear. In recent years various computational approaches have been developed to treat molecules and chemical reactions inside optical cavities at different levels of accuracy.[4,5] Comparison to experimental results is, however, hindered by the collective nature of polaritons, which makes fully *ab-initio* simulations computationally inaccessible. Significant effort has been devoted to the development of alternative approaches, including multiscale models, model Hamiltonians, and rate theories, each with its own advantages and limitations.[6]

In this talk I will present two approaches that we are developing to account for collective effects in quantum simulations. In the first, we describe the behavior of molecules where the cavity is coupled to an electronic transition. We introduce a collective quantum electrodynamics complete active space self-consistent field method (C-QED-CASSCF) that merges the *ab-initio* QED CASSCF wave function[7] with the Hopfield description of polaritons.[8]

In a second part, we use a tensor network framework to perform the open quantum system dynamics of a model describing a molecular aggregate embedded in solvent and an optical cavity environment. This last approach allows us to simulate the cavity-modified chemical kinetics of a cavity coupled to a vibrational excitation of the molecules.

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N-ELECTRON VALENCE PERTURBATION THEORY FOR ELECTRON-PHOTON SYSTEMS

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Strong light-matter coupling in optical cavities leads to the formation of hybrid light–matter states known as polaritons,[1] enabling the modulation of molecular properties and chemical reactivity through quantum electromagnetic fields. This regime, which lies at the core of polaritonic chemistry, requires theoretical approaches that treat electrons and photons on an equal quantum-mechanical footing. While several quantum electrodynamics (QED) extensions of electronic structure methods have been developed, an accurate and balanced description of both static and dynamic electron correlation in strongly coupled systems remains a major challenge. Single-reference QED methods, such as QED-Hartree–Fock[2] or QED-coupled cluster,[2] are reliable for weakly correlated systems but fail in the presence of strong multireference character. Multiconfigurational approaches, including QED-CASSCF,[3] can capture static correlation but neglect dynamic correlation, limiting their quantitative accuracy. We address this limitation by developing a QED extension of N-electron valence state perturbation theory (NEVPT2).[4] Starting from a Dyall Hamiltonian, we derive the perturbative contributions to describe correlated electron-photon systems under strong coupling conditions.

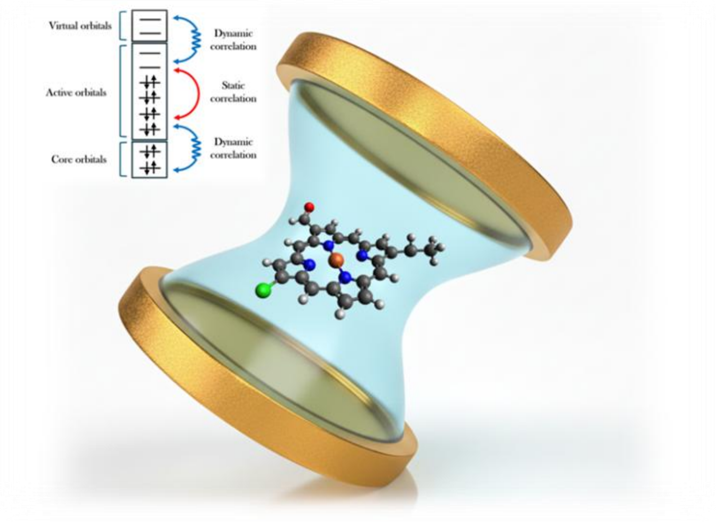

***Figure 1**: Schematic representation of a molecular system inside an optical cavity, highlighting the role of static and dynamic electron correlation within the active, core, and virtual orbital spaces.*

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DEVELOPMENT OF A RELATIVISTIC ONE-DIMENSINAL MODEL INCLUDING QUANTUM ELECTRODYNAMICS EFFECTS

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It is important to take into account the effects of special relativity in the quantum description of chemical systems with heavy elements. The relativistic effects account for gold's color, mercury's liquid state at room temperature and are responsible for the efficiency of lead-acid batteries in cars.[1] Relativistic electronic-structure computational methods have been developed in the no-pair approximation, and are now routinely applied on molecular systems. Hence, the next challenge is to go beyond the no-pair approximation by including the quantumelectrodynamics (QED) effects of virtual electron-positron pairs. Such description is needed to recover some properties, even in very simple systems, e.g. the Lamb shift in the Hydrogen atom. In this work we are interested in a one-dimensional model of relativistic hydrogen-like atom using delta-potential interactions. It is motivated by the non-relativistic version of this model which leads to the same ground-state energy and radial wave function as the three-dimensional one.[2] In this model we are able to make accurate QED calculations.[3,4] After calculating the spectrum of the 1D Dirac operator[5]

$$\mathbf{D}(x) = -\mathrm{i}c\boldsymbol{\sigma}_1\frac{\mathrm{d}}{\mathrm{d}x} + \boldsymbol{\sigma}_3 mc^2 - Z\delta(x)$$

In first quantization, we develop it in a finite basis set. This effective QED theory includes the effects of the vacuum polarization but does not include the photon degrees of freedom.[6,7,8] Within this framework we are able to calculate within a finite basis set the vacuum-polarization density and the QED Lamb-type shift of the bound-state energy.

The next step is to use the insights obtained from simple model to tackle the issues of the 3D case. is it possible for a finite basis set to compute energy shifts coming from divergent quantities?

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EXPLICIT SIMULATION OF CAVITY-QED DEVICES IN POLARITONIC CHEMISTRY: UNRAVELLING THE DEEP NATURE OF THE QUANTUM FIELD-MATTER INTERACTION

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In recent years, the significant progresses made in the engineering and in the fabrication of efficient *optical devices* opened the possibility to use *quantum light* as a new non-invasive tool to control and manipulate the properties of matter. This field is now known (based on the device used and the matter states to which the Quantum Electromagnetic Field couples) as CavityQED[1]/Circuit-QED.[2,3]
Despite Cavity/Circuit-QED attracted the attention of many experimental groups in the past few years, the fundamental origin of the effects induced on matter by quantum light is still debated. In this context, theory represents a complementary tool for understanding crucial aspects of these processes. Among others, allowing to the possibility of optimizing such devices.
In this talk, I will briefly present the *fundamental assumptions* behind the standard state-of-the-art theoretical methods used in polaritonic chemistry, with particular attention to how the choice of gauge influences what we call matter and what we call light.[4] The role of the homogeneous solution of the Maxwell's equations and the concept of zero-point energies, together with the Casimir Effect will be described. Following this logic, two different pictures for explaining the Casimir Effect will be briefly presented: a (formally) simple (but less physical) one, based on the zero-point energy[5] and a (formally) more complicated (but more physical) one based on the general theory of Van der Waals Forces.[6] Aligned with these observations, the rest of the talk will be focused on presenting some of the different approaches we are working on to reformulate *Quantum Electrodynamics* (QED) in terms of Sources.

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