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26 Mar 2026 - 28 Mar 2026
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T01

Superior OER selectivity in bifunctional amorphous cobalt phospho-boride for electrocatalytic seawater splitting

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Utilization of seawater for electrocatalytic water splitting to produce hydrogen and oxygen is a promising yet challenging pathway toward sustainable energy. Conventional water splitting is limited by the scarcity of freshwater resources at large scale, making seawater electrolysis a highly desirable alternative. However, this process requires robust, cost-effective catalysts capable of withstanding the harsh, corrosive environment of seawater—particularly at the anode, where high selectivity for the oxygen evolution reaction (OER) is essential. A significant challenge is the competing oxidation of chloride (Cl^-) ions into various chlorine species, which varies with pH. In this work, we investigated the catalytically active sites of amorphous cobalt phospho-boride, modelled using Car-Parrinello molecular dynamics (CPMD)[1, 2] simulations within the QUANTUM ESPRESSO[3] code. Furthermore, we studied the modulation of active sites through phosphorus incorporation. DFT calculations reveal that phosphorus plays a critical role in optimizing the binding of reaction intermediates by enriching the electron density at the active sites. This mechanism was confirmed through charge transfer and electron localization function (ELF) analyses. These electronic modifications facilitate the OER with high selectivity, providing a sufficient thermodynamic window to suppress the evolution of chlorine-based species. Experimental validation demonstrated low overpotentials of $\approx$270 mV for the hydrogen evolution reaction (HER) and $\approx$410 mV for OER, achieving a current density of 2 $A.cm^{-2}$ at an overall voltage of 2.5 V in highly alkaline natural seawater. These results demonstrate the catalyst's potential for practical, large-scale seawater splitting[4].

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Cu^{2+} Driven Localized Band Formation and Photoluminescence Excitation Splitting in Low Symmetry $Cs_2NaBiCl_6$ Double Perovskite

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Lead-free halide double perovskite (HDP) have attracted great attention as a non-toxic alternative of lead halide perovskites, targeted towards solar energy conversion devices. [1,2] Nevertheless, the major challenge with HDP remains its wide bandgap and low photoluminescence quantum yield which limits their applications.[3] Here, we report Cu^{2+} induced electronic modulation in low symmetry $Cs_2NaBiCl_6$ nanocrystals, synthesized using ligand assisted reprecipitation method. These crystals exhibit orthorhombic Pmmm phase, as compared to the commonly observed Fm-3m phase for $Cs_2NaBiCl_6$.

All our nanocrystals exhibit a pronounced optical absorption peak around 330 nm, corresponding to partially allowed $^1s_0 \rightarrow {}^3p_1$ transition. Upon Cu^{2+} incorporations, we observe a broad optical absorption shoulder emerges at ~390 nm, attributed to dipole forbidden $^1s_0 \rightarrow {}^3p_0$, transition. Though, electronically forbidden ($^1s_0 \rightarrow {}^3p_0$), excitation at 400 nm results into a broad green emission band centred around 515 nm. The emission spectra from both doped and undoped samples have two gaussian contribution in the emission spectra. Their photoluminescence excitation origin is attributed to $^1s_0 \rightarrow {}^3p_1$ and $^1s_0 \rightarrow {}^3p_0$ transitions. Both these, the photoluminescence excitation bands reveal pronounced splitting upon Cu^{2+} doping while the intrinsic $Cs_2NaBiCl_6$ exhibit broad excitation bands. In the intrinsic $Cs_2NaBiCl_6$ host lattice, strong Bi-centred spin-orbit coupling renders the $^1s_0 \rightarrow {}^3p_1$ transition weakly allowed and strongly coupled to lattice vibrations, leading to vibronically broadened excitation and subsequent self-trapped exciton (STE) formation. Upon Cu^{2+} incorporation, localized Jahn-Teller-active Cu-3d states introduce additional ligand-to-metal charge-transfer pathways and impose static and dynamic local symmetry breaking. These effects lift the degeneracy of the excited-state manifold and enhance electron–phonon coupling, resulting in a resolvable multi-component PLE profile.

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Enhancement of Nanowire Solar Cells via Innovative Reinforcement Learning Optimization

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As technology has advanced, the number of parameters involved in system design has grown, making it increasingly difficult to identify optimal solutions. Optimization, a long-standing challenge, aims to find the best solution among many possibilities to maximize system efficiency, performance, and cost-effectiveness. Techniques have evolved from simple parametric sweeps to more sophisticated methods like genetic algorithms and Neuroevolution of Augmenting Topologies (NEAT) [1,2], as well as Particle Swarm Optimization (PSO), which has seen continued refinement over time [3,4]. In recent years, artificial intelligence—especially reinforcement learning (RL)—has emerged as a powerful optimization tool, capable of handling complex, multi-variable problems through continuous learning and adaptation to diverse operational environments [5,6]. This paper introduces a reinforcement learning (RL) optimization framework utilizing a neural network to design high-efficiency nanowire (NW) solar cells (SCs) with modified elliptical geometries. The proposed methodology features a 2×2 array of elliptical NWs with varying shapes to enhance design versatility and degrees of freedom. Initial validation through Finite Difference Time Domain (FDTD) simulations in Ansys/Lumerical achieved a short-circuit current density (Jsc) of 17.6 mA/cm² for a single NW with a 40 nm diameter. Integrating cylindrical NWs with varying diameters in a 2×2 array disrupted mirror symmetry, broadening guided resonances and increasing Jsc by 7.1% to 18.9 mA/cm². Further optimization introduced asymmetrical elliptical-shaped NWs within the 2×2 unit cell, resulting in Jsc improvements of 15.3% and 7% compared to single cylindrical NWs and varied cylindrical NWs, respectively. These findings highlight the RL-driven approach's capability to optimize NW geometries and achieve significant advancements in light absorption and SC efficiency.

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T04

Probing Structural Dynamics of 6 -Methoxyflavone in Different Environments

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Abstract

Environment surrounding the probe reflects the changes in its photophysical behavior. The variations that most affect the fluorescence emission of a probe are usually related to changes in polarity, rigidity, or specific reactions with the fluorophore. Dynamics of solvation and specific interaction of the solute with solvent molecules are of utmost importance in context to elucidate the governing excited state process such as CT, hydrogen bonding, protonation etc. [1]. In the present study, an in-depth photophysical analysis of 6-Methoxyflavone (6MF), using steady-state spectroscopy and lifetime measurements across various solvents and polymers have been performed. Findings reveal that key spectral parameters are highly sensitive to both the polarity and hydrogen-bonding characteristics of the solvent. It has been observed that viscosity exerts a measurable influence on both the steady-state and time-resolved properties of 6MF. In aqueous solution, steady-state and transient data indicate the coexistence of hydrogen-bonded and protonated species. Meanwhile, in aprotic solvents, excitation-dependent spectral behavior appears to stem from conformational and geometrical changes in the molecule. These spectral features make 6MF an efficient probe for the detection of halides and acidic strength [2-3].

Furthermore, 6MF proves to be a sensitive sensor for polymer microenvironments: parameters like polarity, proticity, and free volume significantly affect its fluorescence. In synthetic polymers, whose heterogeneous environments serve as simplified models for more complex biological systems-organic molecules interactions, with these hosts often alter photophysical and photochemical behaviours. Such effects are directly tied to micro-environmental factors. These insights carry important implications for the development of advanced polymer-based materials, especially in photonics and electronics. As the demand grows for novel materials: such as organic thin-film transistors, memory devices, and increasingly miniaturized electronics, understanding and development of these micro-environmental effects becomes vital for innovation and integration.

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Ageing-driven formation of ternary phase N/TiO_2 nanocrystals for sustainable visible-light catalysis

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The ever-increasing energy crisis and environmental pollution have threatened humanity in the past several decades; in this regard, advanced oxidation processes have been extensively explored. Particularly, N-doped TiO_2 nanomaterials have received considerable attention; although, their capability of effectively separating the photogenerated charge carriers substantial improvement [1]. Now days rather than preparing mono-phase nanomaterials (of either Anatase (A), Brookite (B) or Rutile (R)), preparing their mixed-phase TiO_2 nanostructures has been widely considered as the most promising strategy for quantum efficiency enhancement [2]. Nevertheless, reports on ABR triphasic N/TiO_2 nanocomposites are extremely rare due to the fact that their preparation techniques are challenging- follows multi-step reaction under high temperature, which damages their structure and texture properties. Furthermore, the formation of oxygen vacancies, low N-dopant level, and usage of toxic hydrazine/ammonium fluoride as dopant source are the other challenges [3]. Thus, developing a facile preparation method for tunable triphase N/TiO_2 at lower energy simultaneously minimizing the impact on the environment remains quite pivotal. In an open literature survey, most investigations focused on the effect of N-dopant, temperature, surfactant, and solvent type/concentration; the obtained nanomaterials were aged mostly for 1-2 days. The effect of aging time on crystal structure, phase composition, morphology, optical response and photocatalytic activity of N/TiO_2 nanomaterials is overlooked.

Guanidinium chloride is a benign amine; despite its huge N-content, it is barely used as N-dopant source. In the present work with a special focus on aging synthesis approach, we report for the first time its usage in preparing various ABR ternary heterojunction N/TiO_2 nanoparticles at low temperature. Systematically varying the aging time (1, 4, 8, and 12 days), its influence on physicochemical properties of as-obtained spherical heterojunction nanomaterials was studied. Detailed characterizations confirmed that a substantial amount of anatase (88% to 50%) was transformed to rutile (2% to 38%) via intermediate brookite phase (9% to 25%) as the function of aging time; not only the ABR phase content of the samples was tuned by sol-gel age of the precursors but also their optical-response and methylene blue photocatalytic properties were profoundly dictated. Notably under visible-light irradiation, the photostable rutile rich mesoporous triphasic N/TiO_2 (50% A, 12% B, 38% R) aged for 12 days demonstrated higher degradation activity (97%) with a faster degradation rate (0.033 min-1) than both lesser aged N/TiO_2 and undoped titania. This enhancement is attributed to the synergistic effect of interstitial-N-doping and optimal ABR interfacial charge transfer that led to higher light absorption, lower band gap energy and well-separated charge carriers. The current work provides a new perspective for designing highly active visible-light heterostructure nanomaterials with controllable phase composition.

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Taming Light with Carbon dots

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Abstract

The breakthrough of high-power lasers urged the effective light quenching materials for safeguarding eyes, Sensors and Photo detectors. Encountered exploration of Novel carbon dot to manipulate ray of light with a modest price. Nonetheless, a carbon dot suffers a large spectral range detection of a ray of light, so the research has been devoted to exploring the materials to cover different spectral ranges. This article reports a novel multi-photon emissive carbon dot with large spectral emission coverage with an effortless preparation strategy. The rapid fabrication procedure constituted with Multicolour photon emissive carbon dot (MCCD) in a single solvent with utilization of biomass source. We have identified the mono-solvent effect induced Multiple emissive carbon dot observed in fluorescence spectroscopy. The fluorescence carbon particle displays nature of excitation-independent properties, with the granule size ranges 1-15nm result obtained via Transmission Electron Spectroscopy. The carbon structure suffered from the lower carbonization temperature with rapid microwave treatment causing a turbostratic carbon structure. The different colour contains with NIR region bright red emission solution tested against Z-scan non-linear properties, it exposes excited state absorption involved two-photon absorption. It offers an approach for optical limiting behaviour with threshold reaches up to 0.53×10^{-10} and 4.54×10^{12} W/m^2 was observed for MCCD. These results in a gateway for eco-friendly Carbon dot into an optical limiting appeal.

Keywords : *Carbon dots, Psidium gujava, Non-linear optics, Z-scan technique, Triple emission, Microwave assisted method, , Flexible Optical limiters*

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Development and Photoluminescence Spectroscopy study of Luminescent Solar Concentrator for Building Integrated Photovoltaics

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Abstract

Solar energy stands out as a viable renewable source; however, conventional silicon-based photovoltaics exhibit spectral limitations, as they fail to efficiently utilize high-energy UV and low-energy NIR photons, thereby constraining their overall power conversion efficiency. This study aims to enhance solar energy harvesting by integrating upconverting nanoparticles (UCNPs) into luminescent solar concentrators (LSCs) to convert near-infrared (NIR) light into visible light, improving the efficiency of conventional silicon solar cells. Fluoride host matrix $NaYF_4$ co-doped with Er^{3+} and Yb^{3+} was synthesized using the hydrothermal synthesis and characterized structurally and optically. The Upconversion Luminescence (UCL) study based on Photoluminescence (PL), Time Resolved Photoluminescence (TRPL) and Quantum yield measurement is reported. $NaYF_4$: Yb^{3+}, Er^{3+} exhibited the highest UCL efficiency due to its low phonon energy, making it an ideal material for Upconversion. The LSC slabs fabricated with these UCNPs in a resin matrix were evaluated for their optical properties using a custom setup. The findings suggest that $NaYF_4$ based LSCs are particularly promising for enhancing solar energy conversion in building-integrated photovoltaics (BIPV), offering a path toward more sustainable energy solutions.

Keywords: Luminescent Solar Concentrator, Energy harvesting, BIPV,PL,TRPL, Quantum Yield

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T08

Designing all-in-one nanophosphor for thermometry, dosimetry, bioimaging, Anticounterfeiting & X-ray scintillation.

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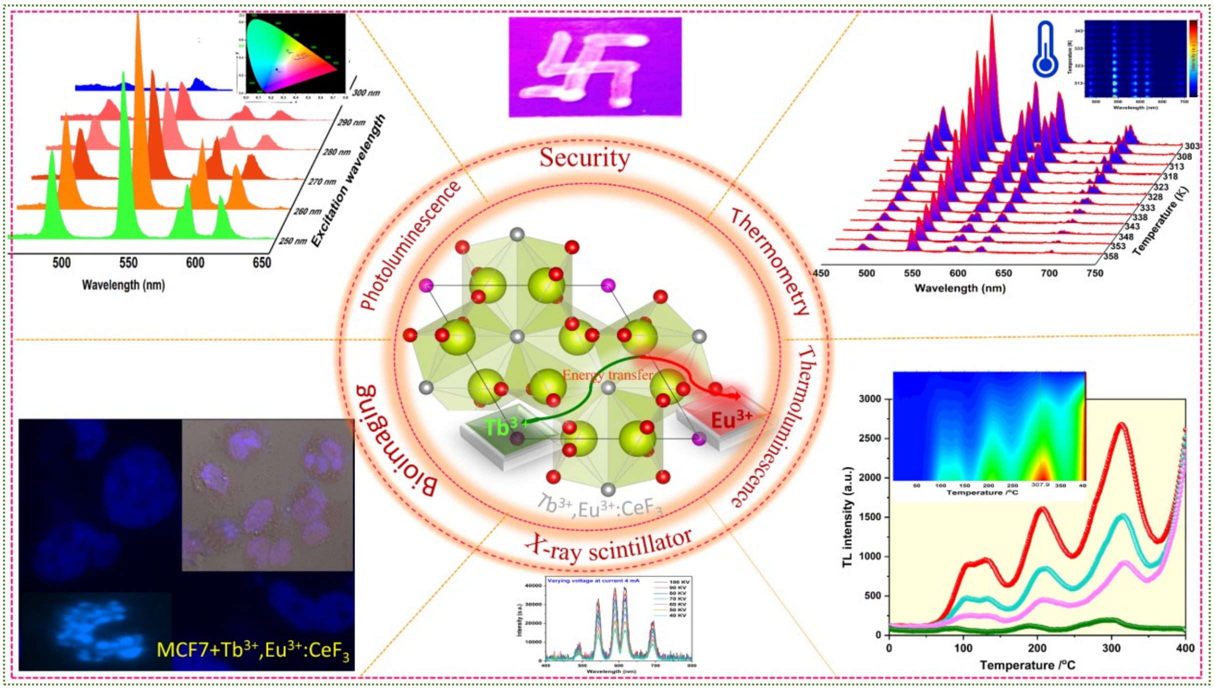
Designing customizable, cost-effective optical material excitable to UV-Vis, X-ray, and β-irradiation (^{90}Sr/^{90}Y) is pivotal for technical innovation and a sustainable society. Engineering a single phosphor for multiple applications is challenging and crucial for innovative technology, elevating productivity and flexibility, minimising cost and power intake, etc. The present work focuses on green synthesis of multifunctional nanophosphor exhibiting versatile optical functionalities. The Unique optical behaviour of the material has shown radioluminescence (RL), photoluminescence (PL), thermoluminescence (TL), scintillation and optically stimulated luminescence (OSL), making it indispensable for X-ray to visible light conversion, fit for biological studies, anticounterfeiting and luminescence thermometry. RL study has shown linear intensity dependence on X-ray tube current 1-5 mA at 100 KV and Voltage 40-100 KV at 4mA, demonstrating efficient X-ray to visible light conversion. The fluorescence intensity ratio technique has shown a maximum relative sensitivity of 1.049%K^{-1}. Biological studies using the MTT assay demonstrated selective cytotoxicity towards MCF7 cells rather than A549 cells. The study reveals that materials exhibit thermal stability, customizability, multicolour tunability, and promising optical properties that are significant for dosimetry, lighting, security, theranostics, anticounterfeiting, thermometry, and bioimaging[1].



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T09

Emergent Excitonic Physics and Interlayer Coupling in Bubble-Free hBN-Encapsulated TMDC Heterostructures

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Two-dimensional (2D) transition metal dichalcogenides (TMDCs) are emerging as a versatile platform for next-generation optoelectronic, photonic, and quantum devices due to their strong excitonic effects, spin–valley coupling, and layer-dependent band structure. However, interfacial contamination, bubbles, and strain in fabricated heterostructures often obscure their intrinsic properties, limiting device performance. Here, we introduce a novel hBN-assisted encapsulation strategy for CVD-grown TMDCs that combines high-temperature processing with an inclined substrate geometry, termed the Hot Inclined Touchdown (HITD) method. This technique leverages the strong adhesion between TMDCs and hBN to achieve clean lift-off from SiO_2 substrates without harsh chemicals, removing interfacial contaminants and minimizing defects. Using this approach, we assemble high-quality homo- and heterobilayers, including MoS_2/MoS_2, WSe_2/WSe_2, and $WSe_2/MoSe_2$, which exhibit narrow excitonic linewidths, enhanced photoluminescence, pronounced interlayer Raman modes, and spatially indirect excitons, demonstrating strong interlayer coupling. Our method provides a scalable route to atomically clean vdW heterostructures, enabling both fundamental excitonic studies and advanced 2D optoelectronic and quantum devices.[1]

[1] Enhanced Excitonic and Interlayer Coupling in Bubble-Free hBN/TMDC Heterostructures, Sudipta Majumder, Rahul Chand, Pradeepa H L, Meghasree Basu, Avinash Mahapatra, Sweta Verma, Sagnik Chatterjee, Kenji Watanabe, Takashi Taniguchi, GV Pavan Kumar, Atikur Rahman. (Under Review)

HARNESSING ARTIFICIAL INTELLIGENCE FOR ENHANCED PHOTOPHYSICAL AND PHOTOCHEMICAL SYSTEMS: PATHWAYS TO SOLAR ENERGY CONVERSION AND PHOTOELECTROCHEMICAL CO_2 REDUCTION

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This poster presents an interdisciplinary approach that leverages advanced artificial intelligence and machine learning techniques to accelerate innovation in photophysical and photochemical research, focusing on applications such as solar energy conversion and photoelectrochemical CO_2 reduction. Building on two decades of experience in computer science and AI-driven data mining across healthcare, environmental, and scientific domains, the work proposes AI-enabled predictive modeling, generative design of photocatalytic materials, and autonomous experimentation platforms. Deep learning architectures are shown to predict and optimize light-matter interactions, guide synthesis of efficient photovoltaic molecules, and interpret complex spectroscopic datasets to foster rapid discovery. The poster highlights workflow examples including inverse design for photoactive materials and ML-assisted catalyst screening for environmentally critical applications. Overall, this research demonstrates how integrating AI/ML with photophysical/photochemical systems accelerates discovery, fosters sustainable energy breakthroughs, and exemplifies cross-disciplinary collaboration within computational and physical sciences.

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Band Alignment and Optical Response in BN- and BP-Based MX_2 (M = Mo, W; X = S, Se) Heterostructures Toward Photocatalytic Water Splitting

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Two-dimensional (2D) van der Waals heterostructures have emerged as promising platforms for photocatalytic water splitting owing to their tunable electronic structure and efficient interfacial charge separation. In this study, we investigate the water-splitting potential of 2D/2D heterostructures formed by hexagonal boron nitride (BN) and boron phosphide (BP) combined with transition metal dichalcogenides MX_2 (M = Mo, W; X = S, Se), including BN/MoS_2, BN/$MoSe_2$, BN/WS_2, BN/WSe_2, and the corresponding BP-based systems.

First-principles density functional theory calculations are employed to construct lattice-matched heterostructures and to examine their structural stability using van der Waals corrected exchange correlation functionals. The electronic structure is analyzed through band structure and density of states calculations, with band edge positions referenced to the vacuum level to evaluate thermodynamic alignment with water redox potentials. Interfacial charge redistribution and electrostatic potential profiles are examined to assess charge separation characteristics and to identify favorable type-II or Z-scheme band alignment. Optical properties are investigated via dielectric function calculations to evaluate visible-light absorption. This study aims to provide fundamental insights into interface-driven electronic and optical properties governing photocatalytic water splitting in BN- and BP-based MX_2 heterostructures.

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Engineering Ce-MOF/$CoFeO_3$ Heterostructures for Enhanced Piezo-Photocatalytic Chromium Reduction and Nitrogen Fixation

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Metal–organic framework (MOF) composites are emerging as promising platforms for light-driven redox reactions due to their structural tunability, high surface area, and ability to interface with functional inorganic phases. In this work, we developed a series of Ce-based MOF/$CoFeO_3$ heterostructures and evaluated their performance as hybrid piezo-photocatalysts under simultaneous visible-light irradiation and ultrasonic mechanical excitation. Structural analysis confirmed successful integration of MOF frameworks (Ce-UiO-66, Ce-MOF-808, Ce-MOF-801) with MOF-derived $CoFeO_3$ nanoparticles without altering the crystalline integrity of the parent MOFs. The resulting heterojunctions exhibited broadened optical absorption (200–550 nm), reduced band gaps, improved charge-carrier separation, and lowered recombination rates, as demonstrated by UV–vis DRS, PL, EIS, and photocurrent measurements.

Among the prepared materials, the $CoFeO_3$/Ce-MOF-801 composite showed the most efficient dual-mode catalytic behavior, achieving 100% Cr(VI) reduction within 30 minutes at pH = 1 and an ammonia production rate of 292.13 μmol g^{-1} h^{-1} L^{-1} in N_2 fixation. Mott–Schottky analysis revealed p–n semiconductor coupling between $CoFeO_3$ and Ce-MOF-801, enabling directional interfacial charge transfer. The synergy between piezoelectric polarization and photoexcitation substantially enhanced electron–hole separation and boosted overall redox efficiency.

These results demonstrate that Ce-MOF/$CoFeO_3$ heterostructures constitute a robust and low-cost class of piezo-photocatalysts with strong potential for applications in environmental remediation and solar-to-chemical energy conversion.

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T13

CO_2 Activation in B- and N-doped C_{20} Fullerene-supported Single-Atom Catalysts – A DFT Study

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Over the past decade, transition metal single-atom catalysts (TM-SACs) have attracted significant attention owing to their promising performance in water splitting, and CO_2 and nitrogen reduction reactions. Carbon-based materials, particularly pristine and heteroatom-doped graphene or carbon nanotubes, are well-recognized supports for TM-SACs. [1] In this work, we propose the C_{20} fullerene nanocage as a novel molecular support for TM-SACs and investigate its potential for CO_2 activation and reduction. TM single-atoms (Ni, Pd, and Pt; denoted as 'M') are anchored on C_{20} (MC_{19}), B- and N-doped C_{20} (MB_2C_{17} and MN_2C_{17}), and B/N-codoped C_{20} ($MBNC_{17}$) to construct a series of SAC models.

Fullerenes are polyhedral carbon cages with the general formula C_{20+2n} ($n \geq 0$, $n \neq 1$) composed of sp^2-hybridized carbon networks. The C_{20} dodecahedral nanocage is the smallest fullerene and, despite being less stable than C_{60}, has been successfully synthesized experimentally by Paquette group et al.[2] Motivated by the reported electrocatalytic performances of fullerene-based systems,[3, 4] we systematically investigate CO_2 adsorption, activation, dissociation to CO* and O*, and the initial pathways of CO_2 reduction reaction (CO_2RR) on pristine and doped C_{20} fullerene-supported TM-SACs.

Density functional theory (DFT) calculations are performed implementing localized orbital basis sets within Gaussian16 package. Structural optimizations of the TM-SACs, with and without adsorbed CO_2 molecules, are carried out using PBE0-D3, B3LYP-D3, ωB97XD, M06-2X, and HSE06 functionals. LanL2DZ effective core potentials are employed for the transition metal atoms, while the 6-311+G(d,p) basis set is used for the lighter elements. Dynamic stability of the optimized geometries is confirmed by the absence of imaginary vibrational frequencies, and thermodynamic stability is further validated through ab-initio Born-Oppenheimer molecular dynamics (BOMD) simulations. Metal-support interactions are characterized using Bader’s quantum theory of atoms in molecules (QTAIM), bond orders, and electronic charge transfer analyses.

For all SACs, only physisorption of CO_2 is observed, as evidenced by the nearly linear geometries of the adsorbed CO_2 molecules. Formation energies, HOMO-LUMO gaps, CO_2 adsorption energies, and structural parameters of the adsobed CO_2 molecules show good consistency across the employed functionals, and B3LYP-D3 is therefore adopted for detailed electronic structure and catalytic analyses. The thermodynamics and kinetics of CO_2 dissociation ($CO_2^* \rightarrow CO^* + O^*$) are evaluated, revealing that B-doped systems exhibit the most favorable energetics and lowest activation barriers. Furthermore, the initial steps of the formate and carboxyl pathways are further examined in competition with the hydrogen evolution reaction (HER), providing insights into CO_2RR selectivity toward CO or HCOOH formation. Overall, this study highlights the potential of C_{20}-based nanocages as molecular supports for TM-SACs in electrocatalytic CO_2RR.

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Electron-phonon coupling induced renormalization of electronic properties in a ternary chalcogenide, $FeBi_4S_7$

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We use first-principles simulations to investigate band-gap renormalization in $FeBi_4S_7$, a transition metal bismuth ternary chalcogenide, under uniaxial strain. Our study emphasizes the role of electron-phonon coupling in determining the electronic properties of this quasi-one-dimensional antiferromagnet, which consists of chains of edge-sharing iron-sulphide (FeS_6) octahedra [1–4]. We examine the ground state magnetic structure and the influence of spin-orbit coupling (SOC) on the electronic properties. The ground-state magnetic structure is found to be antiferromagnetic and is in agreement with the experimental observations. While SOC modifies the magnitude of the band-gap, it does not alter the nature of the band-dispersion curves. The application of hydrostatic pressure as well as uniaxial strain induces a structural transition and significantly reduces the band-gap. We compare the band-gap values from ground-state calculations with those obtained from the simulated optical absorption spectrum, confirming the indirect band-gap nature of the material.

The presence of electron-phonon coupling shows a substantial impact on the band structure, leading to band-gap renormalization at different temperatures and strain levels. The strength of this coupling is quantified using the Huang-Rhys factor [5], and the resulting photoluminescence spectra are computed as a function of uniaxial strain. We observe a direct correlation between the electronic band-gaps and the electron-phonon coupling strength, with both quantities varying oppositely under strain. This coupling significantly influences the excited-state properties, particularly in systems where electronic states are strongly coupled with phonon modes. Strong electron-phonon coupling may lead to non-radiative decay processes and reduce exciton lifetimes [6]. These findings highlight the importance of tailoring electron-phonon interactions to optimize photovoltaic efficiency and device performance.

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T15

Atomic-Scale Insights into Passivation and Halide Mixing in 3D and 2D Halide Perovskites

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Some of the key factors for achieving high efficiency and long-term operational stability in metal-halide perovskite optoelectronic devices require precise control over film growth and effective defect passivation strategies. Recently, amino-silane-treated perovskite solar cells have demonstrated exceptional stability.[1] However, the atomic-scale interactions of these silane molecules at perovskite surfaces remain poorly understood. Separately, to enhance efficiency in quasi-2D perovskites, a recent study achieved vertical crystallization by using methylammonium chloride (MACl) additives during precursor processing.[2] However, the absence of detectable I/Cl halide mixing in 3D perovskites raise fundamental questions about such halide mixing in 2D perovskites.

Our density functional theory and ab initio molecular dynamics simulations reveal atomic-scale insights into these performance improvements, shedding light on the mechanisms of silane passivation in 3D perovskites and halide mixing in 2D perovskites. These findings align with the experimental results and offer a deeper structural and mechanistic understanding at the atomic level.

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T16

Rational Design of Electron-Deficient Tricyanofuran HTMs for Stable Perovskite Solar Cells: A DFT-Based Approach

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Two novel tricyanofuran-based hole-transport materials (HTMs), RK7 and RK8—featuring D_1–D_2–A_1 and A_1–D_1–D_2–A_1 molecular architectures, respectively—were designed and computationally investigated. These designs incorporate phenothiazine–triphenylamine (PTZ–TPA, D_1), benzodithiophene (BDT, D_2), and the electron-deficient tricyanofuran (TCF, A_1) units. Their geometric, electronic, and photophysical properties were analyzed using DFT and TD-DFT calculations at the B3LYP/6-31+G(d,p) level. Clear structure-dependent electronic differences between RK7 and RK8 were revealed through comparisons of HOMO–LUMO distributions, fragment-based energy-level alignments, excited-state electron–hole separation, intramolecular charge-transfer (ICT) character, and ground & excited-state dipole moments. Corresponding trends in their spectroscopic signatures are discussed, with particular emphasis on the influence of introducing a second A_1 moiety in RK8. Finally, the computational findings are correlated with preliminary experimental observations from ongoing collaborative studies, providing comprehensive insight into the structure–property relationships that govern the performance and stability of TCF-based HTMs in perovskite solar cells.