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Advances and perspectives in nanoscale materials and optoelectronics

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The realm of optoelectronics is currently undergoing a transformative phase, driven by convergent developments and innovations in the synthesis, characterization, and application of nanomaterials. This editorial highlights a recent collection of articles in *Nanoscale* that exemplify this exciting evolution, showcasing the rapid bridging of fundamental understanding with technological implementation. A recurring theme across these contributions is the meticulous engineering of materials at the atomic and molecular scale, with increasing emphasis on material robustness, scalability, and performance reproducibility as primary design criteria.

Lead halide perovskites stand out as a prominent class of emerging materials for light-emitting diodes (LEDs) due to their unique structural and optoelectronic properties. However, their widespread adoption hinges on addressing the persistent challenge of defects. Jiang *et al.* (<https://doi.org/10.1039/d3nr06547b>) provide a comprehensive review of defect behavior under electrical fields, a critical aspect for optimizing LED performance. Their work delves into the origins and characterization of these defects, their impact on LED efficiency and stability, and the latest advancements in defect passivation strategies for both bulk materials and nanocrystals. Complementing this, Antony *et al.* (<https://doi.org/10.1039/d2nr06509f>) explore surface defects and

their modification in 2D perovskites, materials highly valued for their solution processability in thin films and individual structures, with applications spanning photovoltaics and other optoelectronic devices. Their study innovatively demonstrates how the oxidation state of lead influences the growth of 2D lead halide perovskite crystals, showing that using PbO_2 as a precursor can directly form the perovskite without requiring additional reducing steps. This approach offers new avenues for controlling crystal formation and morphology.

Chirality, an increasingly vital characteristic in nanomaterials, is thoroughly reviewed by Zhang *et al.* (<https://doi.org/10.1039/d4nr03682d>). Their article explores the spectroscopic intricacies of diverse chiral and helical nanomaterials, including transition metal dichalcogenides, perovskites, and metasurfaces. Significant progress in fabricating and assembling low-dimensional chiral materials and architectures has unveiled novel optoelectronic phenomena, such as circularly polarized light emission, spin, and charge flip. These discoveries hold immense promise for applications in quantum information, quantum computing, and biosensing. Despite these advancements, the fundamental mechanisms governing the generation, propagation, and amplification of chirality in these low-dimensional systems remain largely unexplored. The authors highlight the utility of ultrafast chirality-dependent dynamics investigated by helicity-resolved transient absorption spectroscopy in shedding light on these properties.

Beyond fundamental studies, the application of perovskites' surface properties is exemplified by Yi *et al.* (<https://doi.org/10.1039/d3nr03282e>). Their work details the design and synthesis of hierarchical $\text{CsPbBr}_3/\text{TiO}_2$ heterojunctions, presenting them as stable and efficient photocatalysts for visible-light-driven toluene oxidation. This composite, by integrating perovskite nanoparticles onto nanoflower-shaped titania, leverages the combined structural and electronic advantages of both materials, leading to enhanced solar light utilization, improved toluene adsorption, and superior charge carrier separation and transport. This study underscores the importance of rational design in hierarchical heterojunction catalysts for efficient photocatalytic redox reactions.

The concern regarding the toxicity of lead-based perovskites has spurred research into environmentally friendly alternatives. Wu *et al.* (<https://doi.org/10.1039/d3nr00124e>) review recent breakthroughs in lead-free bismuth-based halide perovskite nanomaterials for heterogeneous photocatalysis under visible light. By achieving novel morphologies, well-designed electronic structures, and engineered surface chemical micro-environments, these lead-free alternatives exhibit enhanced photocatalytic performance in crucial areas such as hydrogen generation, CO_2 reduction, organic synthesis, and pollutant removal. Their review comprehensively covers the synthesis, properties, applications, challenges, and future directions of these promising materials.

The versatility of halide perovskites extends to photodetector applications, as demonstrated by Dao *et al.* (<https://doi.org/10.1039/d2nr07008a>). They present highly stable and flexible broadband photodetectors with remarkable photo-response and durability. Crucially, their design is substrate-free, a significant departure from conventional flexible devices. This innovative approach



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reduces manufacturing waste, cost, and weight, making it particularly suitable for applications in wearable electronics and e-skin. The device exhibits competitive responsivity, bending stability, and response times, outperforming many substrate-based counterparts and simplifying the fabrication process.

For broader integration and mass production, autonomous nanomanufacturing is becoming increasingly vital. Sadeghi *et al.* (<https://doi.org/10.1039/d3nr05034c>) have made a significant stride in this direction by achieving autonomous nanomanufacturing of lead-free metal halide perovskite nanocrystals using a self-driving fluidic laboratory. Their innovative approach combines a modular microfluidic platform with machine learning for the continuous and reproducible in-flow synthesis and optimization of lead-free copper-based metal halide perovskite nanocrystals. This automated system allows for rapid exploration of synthesis parameters and the creation of a digital twin model that predicts nanocrystal properties based on synthesis conditions, accelerating discovery and optimization while minimizing waste and cost.

While many of the aforementioned studies focus on solution-based approaches and their applications, other works delve into the fundamental aspects of colloidal systems. For instance, Cosseddu *et al.* (<https://doi.org/10.1039/d2nr06681e>) employed classical molecular dynamics simulations to investigate the behavior of organic ligands on the surface of CdSe nanocrystals. Their findings reveal that ligands preferentially bind to specific facets, particularly where cadmium atoms have lower coordination numbers, thereby stabilizing these regions. Increased ligand mobility in areas with undercoordinated surface atoms leads to structural rearrangements impacting the nanocrystal's properties. Critically, the study uncovers that low-coordinated selenium atoms can spontaneously form detrimental surface hole trap states, which, although capable of self-healing, can be mitigated by increased ligand coverage.

Infrared (IR) emitters represent another promising application for nanocrystals. Vega-Mayoral *et al.* (<https://doi.org/10.1039/d5nr00511f>) explore the

optoelectronic properties of silver sulfide (Ag₂S) nanocrystals, focusing on the impact of different surface passivation treatments. Their femtosecond transient absorption spectroscopy study reveals that surface passivation enhances photoluminescence quantum yield by reducing defect-related recombination and improving exciton dynamics, making Ag₂S nanocrystals promising for optoelectronics and nanomedicine. Similarly, Ahmed *et al.* (<https://doi.org/10.1039/d3nr00988b>) investigated the photo-physical and nonlinear optical properties of Er and Yb-doped Cs₂AgInCl₆ perovskite nanocrystals, highlighting enhanced near-infrared emission and highly efficient three-photon absorption, suggesting their potential in eco-friendly optoelectronic devices, optical limiting, and photonic switching.

The influence of size, temperature, and pressure on the optoelectronic properties of CsPbI₃ perovskite nanocrystals is investigated by Vukovic *et al.* (<https://doi.org/10.1039/d2nr06345j>). They observed that smaller nanocrystals exhibit higher photoluminescence quantum yield due to stronger ligand binding and reduced non-radiative recombination. Pressure-dependent measurements reveal a phase-specific transition from the γ -phase to the δ -phase, impacting the optical response. These findings underscore the critical role of particle size in determining the structural and optoelectronic properties of CsPbI₃ nanocrystals for photovoltaics and light emission.

The electronic properties of template-grown CsPbBr₃ nanorods were explored by Avila-Lopez *et al.* (<https://doi.org/10.1039/d3nr06682g>) using dielectric force microscopy. Their research reveals that these nanorods exhibit ambipolar behavior for up to two months, subsequently transitioning to p-type conductivity. A key finding is the enhanced electronic uniformity and nanoscale homogeneity of template-grown nanorods compared to conventional counterparts, indicating that this method can lead to more consistent electronic characteristics beneficial for device performance in light-emitting diodes and solar cells.

The demand for non-toxic, high-quality, and cost-effective nanomaterials for optical applications is addressed by Kim *et al.* (<https://doi.org/10.1039/d4nr02524e>) with their successful growth of Zn₃P₂ quantum dots using In (Zn)P cluster seeds. These quantum dots achieved a remarkable photoluminescence quantum yield of 40% and an average decay lifetime of 74 ns, demonstrating high resistance to thermal quenching and an exciton dissociation energy of 62 meV. These advancements are significant for environmentally friendly photonic materials in optoelectronics.

Highly fluorescent quantum dots also hold promise for lasing applications. Nazar *et al.* (<https://doi.org/10.1039/d4nr04653f>) focus on solution-processed shelled semiconductor quantum dots as alternatives to traditional lasers. These nanoparticles effectively reduce non-radiative Auger recombination, enhancing efficiency and longevity. They have demonstrated effective lasing in various configurations with lower thresholds and energy losses, paving the way for applications in photonic circuits, telecommunications, and medical diagnostics, with future goals including electrically pumped laser diodes and expanded spectral capabilities.

The integration of colloidal nanomaterials into functional devices is also making significant progress. Xu *et al.* (<https://doi.org/10.1039/d4nr04620j>) present a single-step efficient method for assembling ligand-exchanged quantum dots for optoelectronic devices *via* electrophoretic deposition. By combining in-solution ligand exchange with electrophoretic deposition, they created dense PbSe nanoparticle films on various substrates, achieving conformal deposition on textured silicon. The resulting infrared photodetectors exhibi-

ted high responsivity and fast response times, highlighting electrophoretic deposition as a scalable and selective technique that enhances device architecture possibilities.

Transfer printing of perovskite nanoparticles for device fabrication is explored by Kajino *et al.* (<https://doi.org/10.1039/d4nr05088f>). Their work details solvent- and heat-free transfer printing methods for lead halide perovskite nanocrystal self-assembled monolayers using viscoelastic PDMS stamps and controlled surface wettability. This direct printing method demonstrated superior performance in terms of film quality and transfer efficiency compared to dual-layer PMMA approaches, ultimately enhancing the integration of perovskite nanocrystals in nano-optoelectronic devices while addressing their instability issues.

The applicability of nanocrystals extends even to the Internet of Things (IoT). Othman *et al.* (<https://doi.org/10.1039/d4nr00203b>) describe the development of phototransistors using quantum dots sandwiched between graphene layers, achieving high external quantum efficiency and fast response times. The integration of low-cost, solution-processed colloidal nanocrystals into IoT is emphasized, along with a focus on developing non-toxic alternatives like InP and perovskite to replace hazardous materials.

Further advancements in advanced devices are demonstrated by Xu *et al.* (<https://doi.org/10.1039/d4nr03579h>), who discuss a piezoelectric nanogenerator utilizing monoclinic phase CsPbBr₃ nanocrystals in PDMS. This generator achieves an impressive output voltage of up to 50 V, a current of 5.5 μ A, and a power density of 2.5 μ W cm⁻² at 30 Hz with a force of 4.2 N. Its remarkable stability, retaining 98.5% output after 20 days, and excellent thermal and humid-

ity resistance, highlight its potential for cost-effective, high-performance energy harvesting.

Finally, the electronic properties of nanocrystal-based devices are investigated by Cavallo *et al.* (<https://doi.org/10.1039/d5nr00767d>), who examine the impact of gate defects in colloidal quantum dot-based field-effect transistors *in operando* using scanning photoemission microscopy. They found that local gate defects significantly alter the energy landscape, potentially leading to electrical breakdown and inducing long-range modulation of the channel's energy profile. Their study underscores the importance of combining electrical measurements with structural analysis for accurate device assessment. Küstner *et al.* (<https://doi.org/10.1039/d4nr02575j>) further investigate PbS/perovskite quantum dot devices using photoconductive atomic force microscopy, providing high precision measurements of barrier height, built-in voltage, diffusion constant, and ideality factor. Their work reveals that photocurrent dependence on light irradiance follows a power law with an exponent of 0.64 and explores the effects of ligands and substrate modifications on photocurrent, offering significant insights into nanostructured hybrid optoelectronic components.

As nanomaterials research continues to mature, it increasingly embodies both scientific ambition and societal responsibility. Future directions in this dynamic field are likely to involve programmable self-assembled systems, defect-tolerant semiconductors, neuro-morphic nanodevices, circular materials chemistry, and real-time *in operando* feedback loops powered by artificial intelligence, all contributing to a sustainable and technologically advanced future in optoelectronics.