Editorial for the Special Issue

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Published in:
Advanced Energy Materials

DOI:
10.1002/aenm.202302239

Editorial for the Special Issue: Emerging Energy and Materials Sciences in Halide Perovskites

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Halide perovskite materials have garnered significant attention for their broad range of applications, particularly in energy devices. The unique optoelectronic properties of perovskites, such as their high light absorption coefficient, long carrier lifetime, small exciton binding energy, and tunable bandgap, have led to the development of high-performance perovskite optoelectronic devices, including solar cells, light-emitting diodes (LEDs), and photodetectors. Furthermore, the feasibility of larger-area fabrication promises mass production of perovskite devices. Although poor environmental stability and the toxicity associated with lead in perovskites have been considered drawbacks, significant progress has been made in addressing these issues.

This special issue on halide perovskite materials, organized and edited by Profs. Feng Yan, Yuanyuan Zhou, Maria Antonietta Loi, and Michael Saliba, features six comprehensive review articles and ten research articles covering important topics in the field. The issue focuses on both material science and applications of halide perovskites, including perovskite solar cells (PSCs) and perovskite light-emitting diodes (PLEDs). Insightful research on material properties is expected to result in improved device performance, while the successful application of perovskite materials in PSCs and PLEDs has motivated researchers to explore the unique properties of halide perovskites, leading to new findings in this field in recent years.

Regarding the material science of halide perovskites, some topics such as compositional engineering, morphology modulation and perovskite junctions have attracted much research interests recently. Perovskite nanomaterials have found emerging applications in many fields. Prof. Zhiyong Fan et al. summarizes the recent progress in the synthesis, integration, property characterization, and advanced optoelectronic applications of one-dimensional (1D) metal halide perovskite nanowires (NWs). This review highlights that metal halide perovskite NWs have advantages over their thin-film counterparts in terms of materials stability and advanced optical properties, making them a research focus in the field of next-generation semiconductor nanomaterials (article number 2201735). Considering the importance of developing perovskite homojunctions and heterojunctions to tune carrier transport properties in optoelectronic devices, Prof. Shihe Yang et al. reviews the recent development of perovskite–perovskite interfaced structures, highlighting the feasible strategies to achieve perovskite junctions and the effects in devices (article number 2201472). Chirality is a property that arises from the structural geometry of materials, which gives rise to unique energy band structures and interesting optical, electronic, and spintronic properties. Halide perovskites have recently been the focus of chirality study and applications due to their large chemical diversity. Professor Yuanyuan Zhou and his colleagues provides a summary of the hierarchical factors contributing to the chirality of halide perovskites. These factors include intercalation, substitution, and distortion at the intra-crystal level, as well as modification at the crystal interface level, and micro-design beyond the crystal level. The review article offers perspectives on both the challenges and opportunities associated with leveraging the chirality present in halide perovskites for device applications (article number 2200792).

Moreover, several research articles on perovskite material science are included in the special issue. The material compositional engineering can lead to tunable structure and optimized optoelectronic properties of halide perovskites. For example, mixed lead-tin halide perovskite is a promising candidate as the bottom subcell of all-perovskite tandem photovoltaics due to its small bandgap while the poor stability of the material in air is a major drawback for photovoltaic applications. Prof. Laura M. Herz et al. investigated the degradation pathway of mixed lead-tin halide perovskite in ambient air and found that the major mechanism can be attributed to the formation of deep trap states (e.g., tin interstitials and iodide vacancies) that are charge neutral, and therefore special passivation strategies for mixed lead-tin perovskites should be developed (article number 2200847). The mixture of two-dimensional/three-dimensional (2D/3D) perovskites

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The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/aenm.202302239

DOI: 10.1002/aenm.202302239

has been developed to improve material stability. Prof. Ana Flávia Nogueira et al. found that bulky cations play important roles on the formation of quasi-2D phases, leading to different formation dynamics and compositions of 2D/3D interface (article number 2201490). Methylammonium has been regarded to be detrimental to the stability of perovskite devices and the incorporation of non-volatile inorganic Cs in methylammonium-free halide perovskites has the potential to increase the material stability. Prof. Mahshid Ahmadi et al. investigated the influence of the amount of Cs in the formation of perovskite phase and found that considerable amounts of non-perovskite phases present in the Cs-rich perovskite at the initial stage of crystallization, which are not completely converted by annealing, whereas a nearly pure, homogeneous α-phase is formed in Cs-moderate perovskite, indicating the importance of controlling the addition of Cs in halide perovskites (article number 2202880).

The investigation of perovskite solar cells has triggered a surge of interest in perovskite optoelectronics. Profs. Shengzhong Liu and Zhike Liu et al. summarize the recent advances in inorganic Cs-based PSCs. This article provides a comprehensive review of advanced strategies for regulating crystal growth of all-inorganic $CsPbX_3$ perovskite, and elucidates the corresponding mechanisms in details. Challenges and commercial applications of such devices are addressed (article number 2201733). Prof. Feng Yan et al. review the recent progress of heterojunction engineering in PSCs. Advanced heterojunction design is of significance to the performance enhancement in PSCs. This review mainly describes the basic physics of heterojunction designs in perovskite solar cells and summarizes different techniques to engineer the charge transport layer /perovskite and perovskite/perovskite heterojunction interfaces with focuses on energy-band alignment optimization, interfacial contact and charge collection improvement, and interfacial trap passivation (article number 2201436). Profs. Xing-Zhong Zhao and Qidong Tai et al. review the recent progress of carbon-based inorganic PSCs. Due to the poor stability of organic-inorganic hybrid PSCs, there has been growing interest in carbon-based inorganic PSCs, which can address the stability challenges by virtue of the absence of organic components. The use of hydrophobic carbon materials as hole transport layers and back electrodes not only simplifies the fabrication process and reduces costs, but also provides protection against moisture erosion. The article summarizes a series of strategies to improve the performance of these devices (article number 2201320). There are four research articles focusing on the device fabrication technique of PSCs. Prof. Letian Dou et al. report the strategy to control the crystallization of Quasi-2D PSCs by introducing bulky conjugated ligands. The authors developed a solvent system that can induce fast surface nucleation and suppress bulk nucleation of perovskite films, leading to improved device efficiency and excellent stability in moisture (article number 2201501). Prof. Yueh-Lin Loo et al. report the construction of ultraviolet (UV)-absorbing transparent PSCs, which are attractive to low-power applications with excellent aesthetics due to their high transparency and color neutrality. The obtained devices based on $CsPbCl_{2.5}Br_{0.5}$ as the absorber exhibit a record average visible transmittance, a high color rendering index, and a promising output power density (article number 2200402). Large-area fabrication of PSCs is critical to the commercialization of the devices. Prof. Eva Unger et al. report the ink design to enable slot-die coating of large-area PSCs. They found that adding lower boiling point solvent acetonitrile to $FAPbI_3$ perovskite precursor inks based on 2-methoxyethanol can reduce the viscosity of the ink, thus changing the solvent removal and crystallization kinetics of the films (article number 2203898). Prof. Seok-In Na et al. report the rheological engineering of supersaturated perovskite ink in the fabrication of slot-die process-based PSCs. By controlling the rheological properties of the ink, uniform perovskite films with dense and large grains have been obtained (article number 2300537).

PLEDs have attracted much attention recently due to the rapidly improved performance and the importance in practical applications. Prof. Thomas D Anthopoulos et al. report perovskite-organic blend LEDs with self-assembled monolayers as hole-injecting interlayers. They observed that additives can effectively modulate the crystallization and growth of perovskite layer and reduce the nonradiative recombination. Moreover, self-assembled monolayers are observed to be favorable for hole injection in LEDs and result in performance improvement (article number 2201396). Prof. Biwu Ma et al. reported the PLEDs based on $CsPbBr_3$ nanoplatelets. The authors introduced an organic sulfate into perovskite precursors, which can passivate the perovskite surfaces and prevent the aggregation and degradation of nanoplatelets during purification and film formation processes, leading to improved photoluminescence quantum efficiency and stability of blue PLEDs (article number 2201605). Prof. Feng Gao et al. present a research article on the impacts of the lattice strain on PLEDs. They found that the lattice strain in perovskite films has negligible relation to the peak efficiency but a strong correlation with device stability. Additionally, increased lattice strain is observed after the device is subjected to a long-term stability test, suggesting that the degradation of the local perovskite lattice structure could be a degradation mechanism for the long-term stable PLEDs (article number 2202185).

The objective of this special issue is to explore the latest advances in perovskite materials and optoelectronics and promote interdisciplinary collaboration worldwide across various fields. The guest editors would like to extend their sincere gratitude to all the authors, reviewers, and the editorial team of AENM, led by Dr. Lulu Ma, for their generous support and dedication to this special issue.

