Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

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Scope of Research

We design and synthesize unique electronic materials with sophisticated device applications in mind. These materials have novel solid-state aggregation structures or well-defined interface orientation that promote efficient electrical current flow or enhance device lifetime. Electronic devices based on these new materials are then evaluated using advanced measurement techniques, and the results are used to inform the next direction of the materials chemistry. We call this synergistic approach for achieving our research goals "Needs Inspired Fundamental Science".

KEYWORDS

Molecular Design and Synthesis Molecular Aggregation Functional Materials Semiconductors Perovskite Solar Cells

Recent Selected Publications

Hu, S.; Pascual, J.; Liu, W.; Funasaki, T.; Truong, M. A.; Hira, S.; Hashimoto, R.; Morishita, T.; Nakano, K.; Tajima, K.; Murdey, R.; Nakamura, T.; Wakamiya, A., A Universal Surface Treatment for p-i-n Perovskite Solar Cells, *ACS Appl. Mater. Interfaces*, **14,** 56290-56297 (2022).

Nakamura, T.; Otsuka, K.; Hu, S.; Hashimoto, R.; Morishita, T.; Handa, T.; Yamada, T.; Truong, M. A.; Murdey, R.; Kanemitsu, Y.; Wakamiya, A., Composition-Property Mapping in Bromide-Containing Tin Perovskite Using High-Purity Starting Materials, *ACS Appl. Energy Mater.*, **5,** 14789-14798 (2022).

Murdey, R.; Ishikura, Y.; Matsushige, Y.; Hu, S.; Pascual, J.; Truong, M. A.; Nakamura, T.; Wakamiya, A., Operational Stability, Low Light Performance, and Long-Lived Transients in Mixed-Halide Perovskite Solar Cells with a Monolayer-Based Hole Extraction Layer, *Sol. Energy Mater. Sol. Cells*, **245,** 111885 (2022).

Hu, S.; Otsuka, K.; Murdey, R.; Nakamura, T.; Truong, M. A.; Yamada, T.; Handa, T.; Matsuda, K.; Nakano, K.; Sato, A.; Marumoto, K.; Tajima, K.; Kanemitsu, Y.; Wakamiya, A., Optimized Carrier Extraction at Interfaces for 23.6% Efficient Tin-Lead Perovskite Solar Cells, *Energy Environ. Sci.*, **15,** 2096-2107 (2022).

Optimized Carrier Extraction at Interfaces for 23.6% Efficient Tin–Lead Perovskite Solar Cells

Carrier extraction in mixed tin–lead perovskite solar cells is improved by modifying the top and bottom perovskite surfaces with ethylenediammonium diiodide and glycine hydrochloride, respectively. Trap densities in the perovskite layers are reduced as a result of surface passivation effects and an increase in film crystallinity. In addition, the orientated aggregation of the ethylenediammonium and glycinium cations at the charge collection interfaces result in the formation of surface dipoles, which facilitate charge extraction. As a result, the treated mixed tin–lead perovskite solar cells showed improved performance, with a fill factor of 0.82 and a power conversion efficiency up to 23.6%. The unencapsulated device also shows improved stability under AM1.5G, retaining over 80% of the initial efficiency after 200 h continuous operation in inert atmosphere. Our strategy is also successfully applied to centimeter-scale devices, with efficiencies up to 21.0%.[1)]

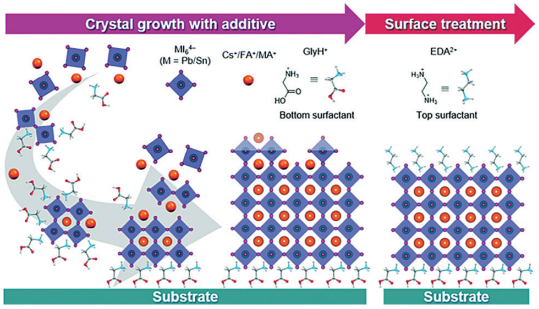

Figure 1. Tin-Lead perovskite films with top and bottom interface modification.

Operational Stability, Low Light Performance, and Long-Lived Transients in Mixed-Halide Perovskite Solar Cells with a Monolayer-Based Hole Extraction Layer

Due to their tunable bandgap and low manufacturing cost, metal halide perovskite solar cells are attractive for ambient/indoor light-harvesting applications. In this work, we evaluate p-i-n perovskite solar cells fabricated with MeO-2PACz, a molecular monolayer hole extraction layer, as potential candidates for ambient light- harvesting applications. Two triple-cation mixed halide lead perovskite absorbers are compared, one with high bromide content (Br/I ratio 1:2, bandgap 1.72 eV, 16.1% power conversion efficiency) and one with low bromide content (Br/I ratio 1:11, bandgap 1.57 eV, 19.1% power conversion efficiency). Both materials demonstrated good stability while operating under simulated sunlight at the maximum power point for 100 h, a cumulative light dose comparable to over two years of ambient use. After 100 h operation, however, the measured device efficiency fell temporarily due to a transient loss of output current before returning to the nominal level after a long recovery period in the dark. These transient losses were more apparent in the wide bandgap device under strong light and were likely caused by light-induced halide segregation. After recovery, both devices retained good performance under a wide range of light intensities. Under a simulated ambient light source (835 lx white LED), the power conversion efficiency of the wide bandgap device reached 30.4%.[2)]

Composition-Property Mapping in Bromide-Containing Tin Perovskite Using High Purity Starting Materials

The wide band gaps of bromide-containing tin perovskites, $ASnI_{3-x}Br_x$, make them attractive materials for use as the top-layer absorber in tandem solar cells, as well as in single junction solar cells for indoor applications. In the present work, a series of $ASnI_{3-x}Br_x$ films was systematically fabricated by varying the A-site (FA^+, MA^+, Cs^+) and X-site (I^-, Br^-) ions. The use of solvent-coordinated $SnBr_2$ complex as a high purity source of bromide combined with Sn(IV) scavenging treatment helps to ensure that the optimal film quality across the compositional space is realized. The energy levels and electronic properties of the films were characterized by photoemission yield spectroscopy and photoluminescence (PL) measurements. The films with long PL lifetime and favorable energy level alignment resulted in superior device efficiency when evaluated in standard single junction solar cells. The best power conversion efficiency of 7.74% was obtained when the composition was $FA_{0.75}MA_{0.25}SnI_{2.25}Br_{0.75}$.[3)]

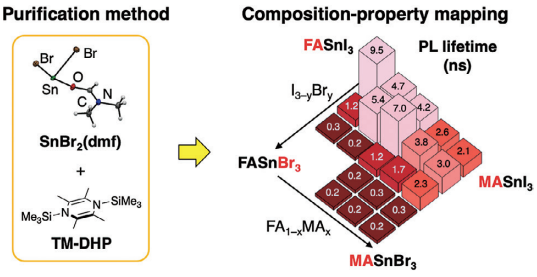

Figure 2. Composition-property mapping in bromide -containing tin perovskite using high purity starting materials.

References

1) S. Hu, K. Otsuka, R. Murdey, T. Nakamura, M. A. Truong, T. Yamada, T. Handa, K. Matsuda, K. Nakano, A. Sato, K. Marumoto, K. Tajima, Y. Kanemitsu, A. Wakamiya, *Energy Environ. Sci.* **2022**, *15*, 2096.
2) R. Murdey, Y. Ishikura, Y. Matsushige, S. Hu, J. Pascual, M. A. Truong, T. Nakamura, A. Wakamiya, *Sol. Energy Mater. Sol. Cells* **2022**, *245*, 111885.
3) T. Nakamura, K. Otsuka, S. Hu, R. Hashimoto, T. Morishita, T. Handa, T. Yamada, M. A. Truong, R. Murdey, Y. Kanemitsu, A. Wakamiya, *ACS Appl. Energy Mater.* **2022**, in press (DOI: 10.1021/acsaem.2c02144).