Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

https://www.scl.kyoto-u.ac.jp/~wakamiya/english/index.html

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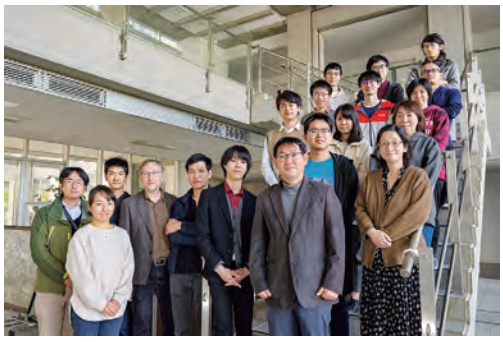
Scope of Research

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
Functional Materials
Perovskite Solar Cells
Molecular Aggregation
Semiconductors

Recent Selected Publications

Jegorovė, A.; Truong, M. H.; Murdey, R.; Daskeviciene, M.; Malinauskas, T.; Kantminiene, K.; Jankauskas, V.; Getautis, V.; Wakamiya, A., Starburst Carbazole Derivatives as Efficient Hole Transporting Materials for Perovskite Solar Cells, *Sol. RRL.*, **6,** 2100877 (2021).

Hu, S.; Truong, M. H.; Otsuka, K.; Handa, T.; Yamada, T.; Nishikubo, R.; Iwasaki, Y.; Saeki, A.; Murdey, R.; Kanemitsu, Y.; Wakamiya, A., Mixed Lead-Tin Perovskite Films with >7 µs Charge Carrier Lifetimes Realized by Maltol Post-Treatment, *Chem. Sci.*, **12,** 13513-13519 (2021).

Cho, Y.; Kim, H. D.; Zheng, J.; Bing, J.; Li, Y.; Zhang, M.; Green, M. A.; Wakamiya, A.; Huang, S.; Ohkita, H.; Ho-Baillie, A. W. Y., Elucidating Mechanisms behind Ambient Storage-Induced Efficiency Improvements in Perovskite Solar Cells, *ACS Energy Lett.*, **6,** 925-933 (2021).

Truong, M. H.; Lee, H.; Shimazaki, A.; Mishima, R.; Hino, M.; Yamamoto, K.; Otsuka, K.; Handa, T.; Kanemitsu, Y.; Murdey, R.; Wakamiya, A., Near-Ultraviolet Transparent Organic Hole-Transporting Materials Containing Partially Oxygen-Bridged Triphenylamine Skeletons for Efficient Perovskite Solar Cells, *ACS Appl. Energy Mater.*, **4,** 1484-1495 (2021).

Near-ultraviolet Transparent Organic Hole-Transporting Materials Containing Partially Oxygen-bridged Triphenylamine Skeletons for Efficient Perovskite Solar Cells

Organic semiconducting materials that are optically transparent in the near-ultraviolet (NUV) region from 300 to 400 nm are needed for advanced perovskite devices such as bifacial semitransparent and tandem solar cells. In this study, three organic semiconducting materials, **HND-NAr$_2$**, **HND-DTP**, and **HND-Cbz**, were designed and synthesized by introducing bis(4-methoxyphenyl)amine, dithieno[3,2-b:2′,3′-d]pyrrole, and carbazole, respectively, into the head position of partially oxygen-bridged triphenylamine skeletons. The combination of oxygen-bridged triphenylamine and an electron-donating group at the head position suppresses the π–π* transition, leading to weak absorption in the NUV region. Thin films of the materials can be fabricated by both solution and vacuum-deposition processes, and applied as the hole-transporting material (HTM) in perovskite solar cells (PSCs). The power conversion efficiency (PCE) of conventional devices with these HTMs was 13.7 % (**HND-Cbz**), 15.0 % (**HND-DTP**), and 17.2 % (**HND-NAr$_2$**). When used in bifacial semitransparent PSCs, the incident photon-to-current conversion efficiency (IPCE) at 400 nm was 41 % (**HND-NAr$_2$**), 45 % (**HND-Cbz**), and 46 % (**HND-DTP**), significantly higher than that of a reference using 2,2′,7,7′-tetrakis(N,N-di-p-methoxyphenylamine)-9,9′-spirobifluorene (spiro-OMeTAD) as the HTM (14 %) as a result of the improved optical transmission through the HTM.[1]

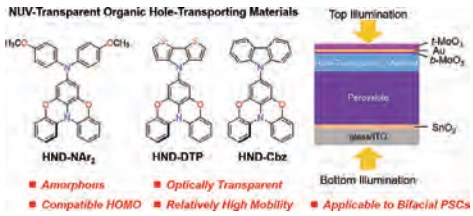


Figure 1. Chemical structures of NUV-transparent organic hole-transporting materials.

Mixed Lead–tin Perovskite Flms with >7 µs Charge Carrier Lifetimes Realized by Maltol Post-treatment

Mixed lead–tin (Pb–Sn) halide perovskites with optimum band gaps near 1.3 eV are promising candidates fornext-generation solar cells. However, the performance of solar cells fabricated with Pb–Sn perovskites is restricted by the facile oxidation of Sn(II) to Sn(IV), which induces self-doping. Maltol, a naturally occurring flavor enhancer and strong metal binding agent, was found to effectively suppress Sn(IV) formation and passivate defects in mixed Pb–Sn perovskite films. When used in combination with Sn(IV) scavenging, the maltol surface treatment led to high-quality perovskite films which showed enhanced photoluminescence intensities and charge carrier lifetimes in excess of 7 µs. The scavenging and surface treatments resulted in highly reproducible solar cell devices, with photoconversion efficiencies of up to 21.4 % under AM1.5G illumination.[2]

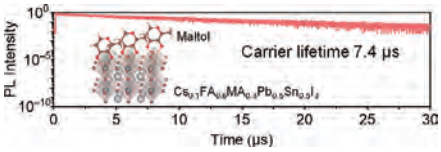


Figure 2. Ultralong charge carrier lifetime of lead-tin perovskite films realized by maltol post-treatment.

Materials Chemistry Approach for Efficient Lead-free Tin Halide Perovskite Solar Cells

The commercial development of perovskite-based photovoltaics is hindered by the toxicity of lead perovskite. Although tin perovskite is a promising alternative, the power conversion efficiency of tin perovskite solar cells has not reached levels comparable to the lead-based devices. Several factors, including the facile oxidation of tin(II) to tin(IV)and difficulties in controlling the morphology of the perovskite layers, are responsible for the lower efficiency. By closely integrating the development of high-purity materials and improved fabrication methods with extensive material characterization, we have been able to improve the performance of tin-based perovskite devices. In this work, highly purified precursor materials for tin perovskites are introduced, together with fabrication methods for pinhole-free and uniform tin perovskite films. The oxidation of tin(II) to tin(IV) during the fabrication process is suppressed by an in situ reducing treatment, which leads to tin perovskite films essentially free from tin(IV) impurities.[3]

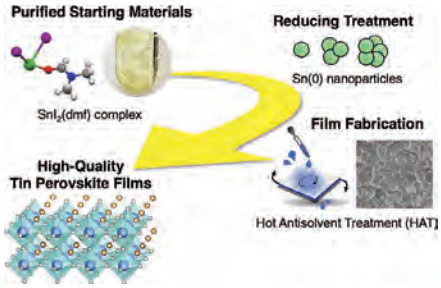


Figure 3. Schematic illustration of the materials chemistry approach for efficient tin halide perovskite solar cells.

References

1) M. A. Truong, H. Lee, A. Shimazaki, R. Mishima, M. Hino, K. Yamamoto, K. Otsuka, T. Handa, Y. Kanemitsu, R. Murdey, A. Wakamiya*, *ACS Appl. Energy Mater.* **2021**, *4*, 1484.
2) S. Hu, M. A. Truong, K. Otsuka, T. Handa, T. Yamada, R. Nishikubo, Y. Iwasaki, A. Saeki, R. Murdey, Y. Kanemitsu, A. Wakamiya*, *Chem. Sci.* **2021**, *12*, 13513.
3) T. Nakamura, T. Handa, R. Murdey, Y. Kanemitsu*, A. Wakamiya*, *ACS Appl. Electron. Mater*. **2020**, *2*, 3794.