高性能ペロブスカイト太陽電池作成に有効な高活性酸化スカベンジャーの開発
Creation of Effective Oxidation Scavenger for Efficient Perovskite-based Solar Cells

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The goal of our collaborative research with Prof. Dr. Atsushi Wakamiya (ICR, Kyoto University) is development of an organic oxidation scavenger for the creation of efficient lead-free perovskite-based solar cells, and pioneering research achievements on the basis of the fusion of elemental science and functional physical chemistry. Challenges for lead-free efficient perovskite-based solar cells such as Sn(II)-based ones compared with their Pb counterparts predominantly include the facile oxidation of divalent Sn(II) into Sn(IV) which leads to the increased nonradiative charge recombination in the perovskite films. Thus, we have focused our research targets on the creation of low-coordinated main group element species as effective oxidation scavengers, which exhibit redox-active property and considerable solubility in organic solvents.

Organostannylenes (R_2Sn:, R = organic substituent) are attractive reactive species, which would exhibit possible ability of working as effecting oxidation scavengers. Isolable organostannylenes remain scarce, and in most hitherto reported examples, the stannylene center is stabilized by electron-donating substituents (e.g., heteroatoms such as nitrogen), which results in electronic perturbation. We have been interested in the chemistry of redox-active stannylenes with carbon-based substituents such as ferrocenyl groups. The reaction of the sterically demanding lithioferrocene (Fc*Li, Fc* = 2,5-bis(3,5-di-t-butylphenyl)-1-ferrocenyl) with SnBr2 afforded the corresponding bis(ferrocenyl)stannylene as a stable crystalline compound. The physical properties such as structural parameters and UV/vis absorptions have been theoretically estimated based of the DFT calculations at B3PW91-D3(BJ)/SDD for Sn, 6-311G(3d) for C, H, Fe level. We are grateful to Prof. Wakamiya (ICR, Kyoto Univ.) for his support on the research, and fruitful discussions.