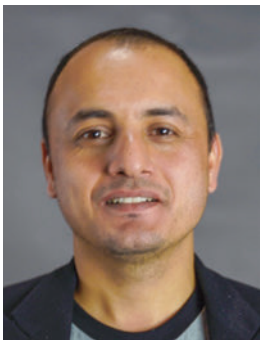
受領No. 1572

擬ハロゲン化物機能性誘導体を用いた高効率・安定な Sn ペロブスカイト太陽電池の開発



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Development of High Efficiency and Stable Sn-perovskite Solar Cells Using Pseudohalide Functional Derivatives

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研究概要

Lead perovskite solar cells (Pb-PSCs) have demonstrated rapid progress in the power conversion efficiency of ~26.1% , as competitive to the prevailed Si-based solar cells. This material, $APbX_3$, is composed of A-site cation, Pb, and X-halogen. The toxicity concern of Pb in Pb-PSCs has imposed barriers to its commercialization application.

To address the toxicity issue, there have been several attempts to replace Pb with non-toxic constituents such as Sn or Bi. Among other candidates, Sn-perovskites (Sn-HP) is the most promising candidate, a close cousin of Pb-halide perovskite. However, this class of material suffers from the facile oxidation of Sn and deteriorates the optoelectronic properties. It is a big challenge to control the oxidation of divalent cations (especially; Sn, Ge-based HP film) and film growth dynamics.

To overcome the issues with Sn-PSC, it is important to modulate the Sn-perovskite material properties and its crystal growth by materials engineering. Here, we propose replacing part of the A and X-site by introducing the polyatomic pseudohalide (X_{PH}) functional derivatives. The alloying at the A and X sites in $FASnI_3$ perovskite with AX_{PH} strengthens the chemical interaction between A-Sn and X-Sn and effectively controls the facile oxidation. We combine the theoretical calculation-guided screening of polyatomic pseudohalide functional derivatives. The objectives of this proposal are (a) optimization of Pb-free (Sn-halide) perovskite film quality using pseudohalide additive, (b) enhancement of device performance and stability, and (c) exploration of device Physics.