SYNTHESIS AND INVESTIGATION OF ORGANIC HOLE SELECTIVE SEMICONDUCTORS WITH DUAL INTERACTIONS AND FUNCTIONALITY IN PEROVSKITE SOLAR CELLS

Gabija Linkaitė[1], Mantas Marčinskas[1], Tadas Malinauskas[1], Vytautas Getautis[1]

[1] Lithuania, Kaunas, Kaunas University of Technology, Faculty of Chemical Technology
gabija.linkaite@ktu.lt

Lead halide perovskites have emerged in recent years as an exceptional semiconductor material used in solar cells and various optoelectronic applications. However, there are still major challenges in the practical application of PSCs, one of which is the toxicity of lead in such perovskites. In order to create lead-free PSCs, one of the possible strategies is to completely or at least partially replace lead with tin. Due to their atomic number, tin-based perovskites could exhibit optoelectronic properties similar to those of their lead-based counterparts. However, the inclusion of Sn^{2+} ions in the perovskite crystal lattice leads to certain undesirable effects: a reduced light absorption coefficient due to a reduced lead content, an inhomogeneous thin-film morphology due to the rapid Sn^{2+} crystallization process, a high defect concentration, a short charge carrier lifetime due to the easy oxidation of Sn^{2+} to Sn^{4+} and high energy barriers at the interfaces. To address these problems, effective strategies have been proposed recently in surface treatments, precursor design, compositional design, and structural optimization, employing various functional materials [1]. Of the many tin-containing perovskite compositions, only Sn-Pb (1:1) perovskite has so far demonstrated promising results close to those of lead-based performance. Since Sn-Pb mixture perovskites have 50% less lead than traditional Pb PSE, the toxicity problem is reduced but not eliminated [2].

In p-type perovskite solar cells, where hole transport layer is formed before the perovskite layer, self-assembled monolayer (SAM) forming compounds were introduced instead of conventional HTMs. SAMs are characterized by good hole extraction properties, higher efficiency, and stability. However, SAMs that show top-tier results in Pb-based PSCs do not replicate these results in Sn-containing PSCs. Not so long ago, a carbazole-based self-assembled monolayer-forming material $BrNH_3$-4PACz was synthesized, which has dual functionality: the carbazole functional group attached to the anchor phosphonic acid group creates a suitable dipole moment on the ITO electrode surface, ensuring optimal energy distribution and effective hole extraction from the narrow bandgap; the ionic ammonium bromide functional group passivates perovskite defects at the surface junction and regulates its crystallization [3]. Due to the dual interaction this compound demonstrated particularly good efficiency in Pb-Sn perovskite solar cells and not so long after was commercialized (by Tokyo Chemical Industry), demonstrating the importance and relevance of such ionic compounds and this concept in general.

In this study, we synthesized and investigated self-assembled monolayer-forming ionic compounds with dual interactions and functionality that could be used to construct Sn-containing perovskite solar cells.

---

[1] W. Gao, F. Yang, Z. Wang, Y. Lan, R. Nie, and C. Ran, "Interface matters: Boosting efficient PB-SN perovskite solar cells for All-Perovskite tandem photovoltaics," Advanced Materials, p. e21789, Jan. 2026, doi: 10.1002/adma.202521789.

[2] H. Lee, S. B. Kang, S. Lee, K. Zhu, and D. H. Kim, "Progress and outlook of Sn–Pb mixed perovskite solar cells," Nano Convergence, vol. 10, no. 1, p. 27, Jun. 2023, doi: 10.1186/s40580-023-00371-9.

[3] S. Zhumagali et al., "Efficient Narrow Bandgap Pb-Sn Perovskite Solar Cells Through Self-Assembled Hole Transport Layer with Ionic Head," Advanced Energy Materials, vol. 15, no. 18, Jan. 2025, doi: 10.1002/aenm.202404617.