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Perovskites with variable bandgap as the basis of new semiconductor materials

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Hybrid organic–inorganic lead-based perovskites have attracted significant attention from the scientific community over the past decade. These compounds have been successfully employed as active-layer materials in solar cells, light-emitting diodes, lasers, and photodetectors. The combination of their outstanding optical and electronic properties, together with the possibility of fabricating them from readily available precursors using simple processing techniques, makes the investigation of semiconductor materials with tunable band gaps, as well as the corresponding quantum dots, highly relevant. It is worth noting that aziridinium-based perovskites represent a rare class of 3D perovskites that are direct-bandgap semiconductors with relatively narrow band gaps. These compounds remain less explored than perovskites containing organic cations such as methylammonium or formamidinium.

In this work, a series of mixed-halide perovskites based on the aziridinium cation was synthesized. Single-crystal X-ray diffraction analysis was employed to determine the halide content and lattice parameters of each sample, as well as to examine the relationship between the perovskite composition and the halide content in the reaction mixture. The band gaps of the obtained materials ranged from 2.33 to 2.95 eV. Additionally, mixed-halide perovskite quantum dots were synthesized and investigated in the course of this study.

[1] Semenikhin, O. A.; Kucheriv, O. I.; Sacarescu, L.; Shova, S.; Gural'skiy, I. A. Quantum Dots Assembled from an Aziridinium Based Hybrid Perovskite Displaying Tunable Luminescence. Chem. Commun. 2023, 59 (24), 3566–3569

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