Structure and electronic properties of morpholinium halide double perovskites: a lead-free hybrid series

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The search for novel organic–inorganic materials combining structural diversity, chemical tunability, and multifunctional behavior is essential for the development of next-generation hybrid materials. These compounds exhibit a wide range of attractive properties, including thermal and environmental stability, structural flexibility, ferroelectricity, and pyroelectric responsiveness. Such functionalities make them highly promising not only for optoelectronic devices like photovoltaics, LEDs, lasers, and photodetectors, but also for applications in non-volatile memory and temperature-sensitive sensors. Among these materials, organic–inorganic hybrids adopting perovskite and double perovskite architectures are of particular interest. The main motivation behind the synthesis of these materials was to introduce additional multifunctionality and structural flexibility that are unattainable in conventional perovskites, limited by the small number of available metal cations. Subsequent studies have demonstrated that such structural and chemical diversity can result in novel materials with previously unobserved, favorable physical properties.

In this study, we report the synthesis and detailed structural analysis of four morpholinium-based lead-free halide double perovskites: $[C_4H_{10}NO]_2[CsBiCl_6]$ (3D, $P2_1/c$), $[C_4H_{10}NO]_2[KBiCl_6]$ (1D, $I2/a$), $[C_4H_{10}NO]_2[CsSbCl_6]$ (3D, $Pca2_1$), and $[C_4H_{10}NO]_2[RbSbI_6]$ (3D, $C2/c$). These compounds were synthesized and characterized using single-crystal X-ray diffraction, revealing how the choice of metal and halide ion influences the resulting dimensionality and symmetry. The influence of cation templating on the resulting framework dimensionality is analyzed, with particular attention given to the consistent 3D architectures found in most compounds and the unique 1D structure observed in one case.

Full structural data and results of density functional theory (DFT) calculations on the electronic properties of these compounds will be presented on the poster.

[1] J. Zhou, et al. *Angew. Chem. Int. Ed.* (2023), **62**,35.

This research was funded by the National Science Centre, Poland, grant number 2021/43/B/ST5/01172.