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First Hybrid Organic-Inorganic Halide Post-Perovskite

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In this work we present a first hybrid organic-inorganic halide post-perovskite $[C_6H_5N_2]PbBr_3$ (Fig. 1a,b) [1]. The crystal structure makes the material anisotropic, what observed in Raman scattering spectra.

The photoluminescence excitation (PLE) and photoluminescence (PL) spectra (Fig. 1c) demonstrate the band gap of the material as 3.25 eV and the broadband emission of self-trapped excitons are the typical features of low-dimensional lead bromide hybrids.

The tilt of inorganic octahedrons along the y -axis creates a tight packing of organic cations in the system. It leads to the appearance of a weak bonding interaction between them and the formation of two uncoupled organic-related bands in the theoretical electronic band structure (Fig. 1d, e). These bands are not flat, but they also do not participate in optical transitions. The band gap is formed by inorganic-related bands, and the calculations show the possibility of both direct and indirect transitions between them.

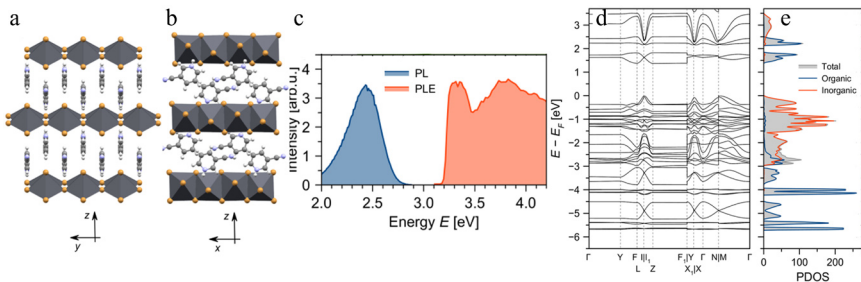


Fig. 1. Crystal structure of $[C_6H_5N_2]PbBr_3$ seen in (yz) (a) and (xz) (b) planes. (c) PL and PLE spectra at $T = 77$ K. Calculated electronic band structure (d) and total density of states (e).

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References

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