Regulation of energy band and luminescence properties in blue quasi-2D lead bromide perovskite via lattice strain

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Abstract: Development of blue quasi-2D lead halide perovskite LEDs is key to the perovskite based full-color displays and white-light

illumination. It is still quite challenging to accurately enlarge the bandgap to achieve high performance and stable blue Quasi-2D perovskite LEDs. The lattice strain due to the deformation of lead-bromide octahedra is a critical factor leading to the energy band adjustment and stability optimization. In this Letter, the lattice strain is adjusted via three cations with different sizes, Cs^+, $CH_3CH_2NH_2^+$ (EA^+), and Rb^+, for sophisticatedly micro-tuning of the lattice strain to achieve overall lattice expansion and lattice contraction. A ternary quasi-2D blue bromide perovskite material $PEA_2(Cs_xEA_yRb_{1-x-y}PbBr_3)_2PbBr_4$ is specially designed. The crystal structure and energy band are studied by the first principles calculations using the Density Functional Theory method. The luminescence properties of blue quasi-2D lead bromide perovskite materials are analyzed with spectra regulation from 508 to 464 nm for photoluminescence and from 510 to 470 nm for electroluminescence. The thermal treatment is used to accelerate the release of residual strain due to mismatch and disorder in the lattice, leading to defects and degradation. The lattice strain is strongly correlated with the energy band, luminescence performance, and thermal stability of blue quasi-2D lead bromide perovskite. The study of lattice strain relaxation in blue quasi-2D lead bromide perovskite could open avenues for high-performance and stable blue quasi-2D perovskite LEDs.

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