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First-principles study of γ-ray detector materials in perovskite halides[1] JINO IM, HOSUB JIN, Northwestern University, CONSTANTINOS C. STOUMPOS, DUCK YOUNG CHUNG, Argonne National Laboratory, ZHIFU LIU, JOHN A. PETERS, BRUCE W. WESSELS, Northwestern University, MERCOURI G. KANATZIDIS, Northwestern University; Argonne National Laboratory, ARTHUR J. FREEMAN, Northwestern University — In an effort to search for good γ-ray detector materials, perovskite halide compounds containing heavy elements were investigated. Despite the three-dimensional network of the corner shared octahedra and the extended nature of the outermost shell, its strong ionic character leads to a large band gap, which is one of the essential criteria for γ-ray detector materials. Thus, considering high density and high atomic number, these pervoskite halides are possible candidate for γ-ray detector materials. We performed first-principles calculations to investigate electronic structures and thermodynamic properties of intrinsic defects in the selected perovskite halide, $CsPbBr_3$. The screened-exchange local density approximation scheme was employed to correct the underestimation of the band gap in the LDA method. As a result, the calculated band gap of $CsPbBr_3$ is found to be suitable for γ-ray detection. Furthermore, defect formation energy calculations allow us to predict thermodynamic and electronic properties of possible intrinsic defects, which affect detector efficiency and energy resolution.

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