Abstract Submitted
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Cs-based gamma-radiation detector material $Cs_2Hg_6S_7$: First-principles study of extrinsic doping[1] JINO IM, SHICHAO WANG, JOHN A. PETERS, ZHIFU LIU, BRUCE W. WESSELS, MERCOURI G. KANATZIDIS, ARTHUR J. FREEMAN, Northwestern University — Semiconductor X-ray/γ-ray radiation detectors have broad applications, yet finding superior detector materials that work at room temperature is a challenge because of its contradictory requirements. In a previous study, the ternary compound $Cs_2Hg_6S_7$ was proposed as a possible candidate because of its high density, optimal band gap and high $\mu\tau$ values. However, the low resistivity originating from p-type carriers is a detrimental factor that limits its performance. As a strategy to increase the resistivity, we investigated compensation by extrinsic doping. Using first-principles density functional theory calculations we focused on finding a proper dopant which gives a shallow donor level that leads to a compensation of hole carriers. We tested a number of extrinsic dopants and, as a result, we found that indium is a promising dopant for the strategy to increase the resistivity of $Cs_2Hg_6S_7$.

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