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First-principles study of γ-ray detectors: Cs-based compounds[1]

HOSUB JIN, JINO IM, ARTHUR FREEMAN, Department of Physics and Astronomy, Northwestern University, BRUCE WESSELS, Department of Materials Science and Engineering, Northwestern University, MERCOURI KANATZIDIS, Department of Chemistry, Northwestern University — In an effort to find good candidate materials for γ-ray detectors, Cs-based compounds containing heavy elements, such as in $Cs_2Hg_6S_7$, were investigated. We performed *ab-initio* density functional theory calculations using the full-potential linearized augmented plane wave method[2]. The screened-exchange local density approximation (sX-LDA) scheme was employed to correct the underestimation of the band gap in the LDA method. As a result, the band gap of $Cs_2Hg_6S_7$ is predicted to be 1.23 eV by sX-LDA, corrected from 0.51 eV by LDA. Therefore, $Cs_2Hg_6S_7$ seems to be useful as a γ-ray detecting material in terms of the high density and the band gap. Not only the pristine bulk but also several defect configurations were calculated, which affects the transport properties. Defect formation energy determinations allow us to predict which defect configuration is most likely in $Cs_2Hg_6S_7$.

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[2]Wimmer, Krakauer, Weinert, Freeman, Phys. Rev. B, **24**, 864 (1981)

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