

Abstract Submitted
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First-principles study of γ -ray detector materials : heavy alkali metal compounds¹ HOSUB JIN, JUNG-HWAN SONG, ARTHUR J. FREEMAN, BRUCE W. WESSELS, MERCOURI G. KANATZIDIS, Northwestern University — In an effort to find good candidate materials for γ -ray detectors, alkali metal based chalcogenide semiconductors containing heavy elements were investigated. We performed ab- initio density functional theory calculations using the highly precise full-potential linearized augmented plane wave (FLAPW) method² to estimate their electronic characteristics. The state-of-the-art screened-exchange LDA scheme was adopted to correct the underestimation of the band gap in the LDA method. Several candidate materials for γ - ray detectors such as $\text{Cs}_2\text{Cd}_3\text{Te}_4$ and $\text{Cs}_2\text{Hg}_6\text{S}_7$ were suggested based on the electronic properties like band gaps, effective masses, absorption coefficients, and work functions. Lattice degrees of freedom such as static dielectric constants and bulk modulus were also calculated, and are reported.

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

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