

Abstract Submitted
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**Electronic structures of Tl-based materials for γ -ray detectors;
First-principles study¹** JUNG-HWAN SONG, HOSUB JIN, ARTHUR J. FREEMAN, SIMON JOHNSEN, JOHN ANDROULAKIS, PETER SEBASTIAN, ZHIFU LIU, JOHN A. PETER, NAM-KI CHO, BRUCE WESSELS, MERCOURI G. KANATZIDIS, Northwestern University — For Tl-based semiconductors, investigated to find good candidate materials for γ -ray detectors, we performed ab-initio calculations using the full-potential linearized augmented plane wave (FLAPW) method² to find their electronic structures and to estimate their physical properties such as band gaps, effective masses, absorption coefficients, dielectric constants, and work functions. Within the LDA scheme, the underestimation of the band gap is well-known and causes serious problems in obtaining optical properties. Therefore, we adopted the screened-exchange LDA (sX-LDA) scheme and acquired correct gap values close to experimental ones. With the sX-LDA, we found that $\text{Tl}_6\text{I}_4\text{S}$ and $\text{Tl}_6\text{I}_4\text{Se}$ have direct band gaps of 2.36 and 1.88 eV, respectively, and they exhibit dispersive bands near the band edges. Based on the calculated and experimental results, we discuss the relationship between atom species/crystal structure and electronic characteristics, and suggest several materials for γ -ray detectors.

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

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