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Electronic structure and defect properties of hybrid chalcohalides $Hg_3Q_2I_2$ (Q=S, Se and Te) for radiation detection[1] OLEG Y. KONTSEVOI, YIHUI HE, BRUCE W. WESSELS, MERCOURI G. KANATZIDIS, Northwestern University — Heavy metal chalcohalides $Hg_3Q_2I_2$ (Q=S, Se and Te) have shown significant promise as X-ray and γ-ray detector materials. To assess the fundamental physical properties important for their performance as detectors, theoretical calculations were performed for the electronic structure, band gaps, electron and hole effective masses, and native defect properties. The calculations were based on first-principles density functional theory (DFT) and employ the highly precise full potential linearized augmented plane wave method and the projector augmented wave method and include nonlocal exchange-correlation functionals to overcome the band gap underestimation in DFT calculations. The calculations show that $Hg_3Q_2I_2$ have either indirect (Q=S, Se) or direct (Q=Te) band gaps within 1.9-2.25 range which is optimal for a detector material, and very small electron effective masses (0.19 m_0 for $Hg_3Se_2I_2$) which could result in a good carrier mobility-lifetime product $\mu\tau$. We further investigated a large set of native defects in the most promising candidate material, $Hg_3Se_2I_2$, to determine the optimal growth conditions for application as γ-ray detectors. The results suggest that the prevalent intrinsic defects are iodine vacancies, mercury vacancies, and selenium vacancies followed by antisite defects. The effect of various chemical environments on defect properties was examined and the optimal conditions for material synthesis were suggested. [1]Supported by DHS (Grant No. 2014-DN-077-ARI086-01).

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