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Electronic structure and defect properties of selenophosphate $Pb_2P_2Se_6$ for γ-ray detection[1] OLEG Y. KONTSEVOI, JINO IM, BRUCE W. WESSELS, MERCOURI G. KANATZIDIS, ARTHUR J. FREEMAN, Northwestern University — Heavy metal chalco-phosphate $Pb_2P_2Se_6$ has shown a significant promise as an X-ray and γ-ray detector material. To assess the fundamental physical properties important for its performance as detector, theoretical calculations were performed for the electronic structure, band gaps, electron and hole effective masses, and static dielectric constants. 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 $Pb_2P_2Se_6$ is an indirect band gap material with the calculated band gap of 2.0 eV, has small effective masses, which could result in a good carrier mobility-lifetime product $\mu\tau$, and a very high static dielectric constant, which could lead to high mobility of carriers by screening of charged scattering centers. We further investigated a large set of native defects in $Pb_2P_2Se_6$ to determine the optimal growth conditions for application as γ-ray detectors. The results suggest that the prevalent intrinsic defects are selenium vacancies, followed by lead vacancies, then phosphorus vacancies and 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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