

Abstract Submitted
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Density functional study of the properties of Tl₆SeI₄ for radiation detection applications KOUSHIK BISWAS, Arkansas State University, MAO-HUA DU, DAVID SINGH, Oak Ridge National Laboratory — The extra compositional freedom available in ternary compounds allow flexibility to tune their electronic and structural properties compared to the binary counterparts. Indeed, the Tl-based ternary semiconductor Tl₆SeI₄ is a promising candidate for radiation detectors. It has a band gap (1.86 eV) that is intermediate between those of Tl₂Se (0.6 eV) and TlI (2.75 eV) and suitable for room temperature detectors. However, the flexibility in ternary semiconductors may come at the expense of more channels for defect formation and more complex defect chemistry, which need to be studied in details. To better understand the properties of Tl₆SeI₄ in relation to the radiation detection, we performed first-principles study of electronic structure, phase diagram, and dielectric, optical, and defect properties in Tl₆SeI₄. [1] We will discuss the properties of defects and their diffusion barriers in the context of resistivity and polarization phenomenon in Tl₆SeI₄. [1] K. Biswas, M.-H. Du, and D. J. Singh, Phys. Rev. B **86**, 144108 (2012).

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