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DFT Studies of Semiconductor and Scintillator Detection Materials

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Efficient radiation detection technology is dependent upon the development of new semiconductor and scintillator materials with advanced capabilities. First-principles based approaches can provide vital information about the structural, electrical, optical and defect properties that will help develop new materials. In addition to the predictive power of modern density functional methods, these techniques can be used to establish trends in properties that may lead to identifying new materials with optimum properties. We will discuss the properties of materials that are of current interest both in the field of scintillators and room temperature semiconductor detectors. In case of semiconductors, binary compounds such as TlBr, InI, CdTe and recently developed ternary chalcohalide Tl6SeI4 will be discussed. Tl6SeI4 mixes a halide (TlI) with a chalcogenide (Tl2Se), which results in an intermediate band gap (1.86 eV) between that of TlI (2.75 eV) and Tl2Se (0.6 eV). For scintillators, we will discuss the case of the elpasolite compounds whose rich chemical compositions should enable the fine-tuning of the band gap and band edges to achieve high light yield and fast scintillation response.