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Electronic properties of BiI3 using hybrid functionals[1] PATRICK M. MCBRIDE, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — BiI3 has recently gained interest as a high-efficiency light-output scintillator material, but limited research has been done to investigate its electronic structure. Most theoretical investigations have been limited to using density functional theory (DFT) within the local density approximation (LDA) or the generalized gradient approximation (GGA), which are known to give an incorrect electronic band gap. Furthermore, these studies ignore van der Waals (vdW) interactions, even though BiI3 has a layered structure held together by vdW forces. In this talk we present results of hybrid functional calculations, including the effects of spin-orbit coupling, for the electronic and structural properties of BiI3. We will address effects of including vdW interactions and spin-orbit coupling on the nature of the band gap, electron and hole effective masses, and the band edge positions with respect to vacuum level and other relevant semiconductors. We will also discuss the suitability of BiI3 as a photovoltaic material.

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