

Abstract Submitted
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Theoretical study of bismuth-doped cadmium telluride¹ E. MENENDEZ-PROUPIN, Universidad de Chile, J. A. RIOS-GONZALEZ, J. L. PENA, CINVESTAV-Unidad Merida — Cadmium telluride heavily doped with bismuth has been proposed as an absorber with an intermediate band for solar cells. Increase in the photocurrent has been shown recently, although the overall cell efficiency has not improved [1]. In this work, we study the electronic structure and the formation energies of the defects associated to bismuth impurities. We have performed electronic structure calculations within generalized density functional theory, using the exchange-correlation functional HSE(w), where the range-separation parameter w has been tuned to reproduce the CdTe bandgap. Improving upon previous reports [2], we have included the spin-orbit interaction, which modifies the structure of the valence band and the energy levels of bismuth. We have found that interstitial Bi (Bi_i) tends to occupy Cd vacancies, cadmium substitution (Bi_{Cd}) creates single donor level, while tellurium substitution (Bi_{Te}) is a shallow single acceptor. We investigate the interaction between these point defects and how can they be combined to create a partially filled intermediate band. [1] O. Vigil-Galan et al, J. Mater. Sci: Mater Electron (2016) 27: 6088. [2] Y. Seminovski et al, Solar Energy Materials & Solar Cells (2013) 114: 99

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