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Tunable optical properties of $ZnCdTe_{2-x}Se_x$ (x = 0.625) chalcopyrite for photovoltaics; a mBJLDA approach [1] MANISH K. KASHYAP, D. PAUDYAL, B. N. HARMON, Ames Laboratory, U.S. Department of Energy, Iowa State University, Ames, Iowa 50011-3020 — In the present study, we have performed ab-initio simulations of sp-element defect in $ZnCdTe_{2-x}Se_x$ (x =0.625) chalcopyrite to check the tuning of band gap as compared to the pristine case. The exchange and correlation (XC) effects are taken into account by an orbital independent modified Becke-Johnson (mBJ) potential as coupled with Local Density Approximation (LDA) for these calculations. The calculated energy band structures show a direct band gap at the point in the brillouin zone for the pristine as well as the defected case and the band gap decreases with inclusion of sp-disorder. The imaginary dielectric function predicts the optical band gap of pristine $ZnCdTe_2$ very close to the experimental value and the results are in reasonable agreement without applying any scissor operator. With inclusion of sp-element defect, the optical spectra is tuned to optimal region, suitable for photovoltaics. It is apparent that mBJ functional is well suited for calculating electronic structure of pristine as well as defected $ZnCdTe_2$ chalcopyrite.

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