Abstract Submitted
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***Ab initio* studies of defects in CdTe and HgTe with symmetrized basis**[1] YIA-CHUNG CHANG, HYEJUNG KIM, University of Illinois at Urbana-Champaign — We have performed *ab initio* pseudopotential calculations of the total energies and atomic realxations of neutral and charged Cd vacancies in CdTe and Hg vacancies in HgTe. Our method takes advantage of the high point symmetry of the system, which enables us to use large supercells containing up to 64 atoms per unit cell. Supercells of 8, 16, 32, 54, and 64 atoms are employed and spin-orbit interactions are included. Considering only symmetric relaxations of neighboring atoms in CdTe system of a 64-atom supercell, we find that first-neighbor atoms around a Cd vacancy move toward the vacancy with a 9% contraction in bond length and second-neighbor atoms move toward the vacancy with a 2.5% lowering contraction in inter-atomic distance. The relaxation lowers the total energy by about 0.2eV. Similarly in HgTe, the contractions are 7% and 1.5%, respectively for first-neighbor and second-neighbor atoms. Three defect levels (with symmetryΓ_6,Γ_7, andΓ_8) are found for both CdTe and HgTe systems and one of the levels is located in the band gap while two of them are buried under the valence band maximum. Separate calculations are carried out using a full potential linearized augmented Slater-type orbital (LASTO) method and give consistent results. Self-energy corrections due to many-body effect are also estimated with the GW approach.

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