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First Principles Investigation of H in CdTe HIROYUKI TAKENAKA, DAVID J. SINGH, MAO-HUA DU, Oak Ridge National Laboratory — CdTe and alloys particularly (Cd,Zn)Te are of interest for radiation detection and other applications. A key issue is obtaining high mobility compensated material with low concentrations of traps. Hydrogen has been shown to play an important role in various semiconductors with both beneficial and deleterious effects. We investigate the effect of H on vacancies in CdTe using supercells. Our results are obtained from the first principles density functional theory calculations using the full potential linearized augmented planewave method including local orbitals and based on local density approximation. H atoms in Cd vacancies move toward one of Te atoms, which form Td symmetry with Cd in the bulk system. The bond length between H and Te is 1.7 angstrom. This corresponds to a closely bonded Te-H unit similar to OH. We also present H in Te vacancies. We report the electronic structures as well as positron lifetimes. This work was supported by DOE, NA-22.

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