Self-compensation of group-V acceptors in CdTe

Anderson Janotti, Intuon Chatratin, Igor Evangelista
Department of Materials Science and Engineering, University of Delaware, Newark, DE, United States

Cadmium Telluride is at the core of an important thin-film technology for photovoltaics that is already commercially available, yet the CdTe-based solar cell efficiency remains limited at 22%, well below the theoretical limit of ~30%. Increasing the hole concentration is crucial for higher efficiency, and group-V elements such as As, P, and Sb are potential dopants as they are shallow acceptors. Nevertheless, group-V doped *p*-type CdTe often exhibits low doping activation, and the compensation source remains debated. Here, we performed hybrid density functional calculations with spin-orbit coupling to investigate possible sources of hole compensation in group-V doped CdTe. First, regarding possible self-compensation of the group-V dopants, we find that the formation of AX centers is unlikely since they are found to be unstable relative to the shallow acceptor forms. However, if the group-V dopants come in during growth (such as dimer molecules As_2, P_2, and Sb_2), we find that the impurity atoms, which would occupy nearest neighbor sites, maintain the V-V bonds, limiting the hole density. For the native defects, our study reveals that Cd interstitial is the lowest energy donor defect in p-type CdTe. Still, it has a small migration barrier of 0.5 eV, making it highly mobile and unstable at room temperature. The Te vacancy is the next lowest formation energy donor. The migration barrier of 1.4 eV indicates that the Te vacancy is stable at room temperature. The antisite Cd_{Te} is also a donor, with low formation energy and stable at room temperature, potentially limiting the hole concentration. Our results, therefore, shed light on possible compensation centers and some guidance on how to avoid them.

Acknowledgement: This work was supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy (EERE) under Solar Energy Technologies Office Award Number DE-EE0009344.