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First principles investigations of defect-mediated carrier recombination centers in cadmium telluride JIE PAN, WYATT METZGER, STEPHAN LANY, Natl Renewable Energy Laboratory — Cadmium telluride (CdTe) is a leading thin film photovoltaic (PV) material for its low manufacturing cost. To improve the conversion efficiency and open-circuit voltage, it is necessary to investigate the structures and energies of defects in CdTe which can shed lights on the defect-mediated carrier recombination pathways. However, standard density functional theory (DFT) calculations can not accurately describe defect structures in CdTe, especially for the defects with open shells. To overcome this challenge, we developed a Hartree-Fock/DFT hybrid functional that can fully correct the band gap of CdTe. Based on this hybrid functional, we examined the atomic configurations, formation energies, and transition levels of intrinsic defects, impurities (e.g., Cu, Cl), and defect complexes in CdTe. According to the defect levels relative to the band edges in CdTe, the mechanisms of defect-mediated carrier recombination, e.g., radiative, non-radiative, were proposed.

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