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Stacking faults and lamellar twins with intrinsic point defects in poly-crystalline CdTe analyzed by density functional theory CHRISTOPHER BUURMA, Univ of Illinois - Chicago, MARIA CHAN, Argonne National Laboratory, TADAS PAULUASKAS, ROBERT KLIE, SIVALINGAM SIVANANTHAN, Univ of Illinois - Chicago, DOE BRIDGE PROJECT COLLABORATION — Polycrystalline CdTe is a prominent photovoltaic material with proven industry success. To develop the next generation of thin film CdTe solar cells, higher open-circuit voltages and longer minority carrier lifetimes must be achieved. Playing a major role in doping, defect migration, recombination, and current transport are grain boundaries and other extended defects within grains of poly-crystalline CdTe. Commonly observed with STEM in CdTe are twins and stacking faults that extend throughout the entire grain. These twins can appear as lamellar repeating twins, or as single column stacking faults occurring in repetition near that of a Wurtzite structure. In this talk, we will use first principles density functional theory to investigate the thermodynamics and electronic structures such structures observed in STEM. The interaction energetics between adjacent twins and sets of twins are investigated. We will also investigate the likelihood of formation of neutral and charged native point defects in and near these extended defect structures. Binding energies of multiple point defects near such structures are also revealed. Implications towards PV efficiencies are discussed.

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