Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First principles modeling of grain boundaries in CdTe[1] MARIA K.Y. CHAN, FATIH SEN, Argonne National Laboratory, CHRISTOPHER BURMA, EPIR, TADAS PAULAUSKAS, University of Illinois Chicago, CE SUN, MOON KIM, University of Texas at Dallas, ROBERT KLIE, University of Illinois Chicago — The role of extended defects is of significant interest for semiconductors, especially photovoltaics since energy conversion efficiencies are often affected by such defects. In particular, grain boundaries in CdTe photovoltaics are enigmatic since the achievable efficiencies of CdTe photovoltaics are higher in polycrystalline devices as compared to single crystalline devices. Yet, despite recent advances, the efficiency of poly-CdTe devices are still substantially below the theoretical maximum. We carry out an atomistic-level study using Scanning Transmission Electron Microscopy (STEM), together with first principles density functional theory (DFT) modeling, in order to understand the properties of specific bicrystals, i.e. artificial grain boundaries, constructed using wafer bonding. We discuss examples of bicrystals, including some involving large scale DFT calculations, and trends in defect and electronic properties.

[1]This work was funded by DOE SunShot BRIDGE program.

Maria K.Y. Chan
Argonne National Laboratory

Date submitted: 22 Jan 2016 Electronic form version 1.4