Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-principles studies of structure and electronic level alignment at nanoscale CdSe/CdTe heterojunctions[1] SHENYUAN YANG, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Group II-VI semiconductor nanostructured heterojunctions with type-II interfacial band offsets have many potential applications in nanoscale optoelectronics and photovoltaics. A key open question is how the electronic level alignment at nanoscale heterojunctions differs from that at their bulk counterparts, and whether bulk intuition can be used to understand their electronic behavior. We use density functional theory and beyond to study the structure and electronic properties of CdSe/CdTe interfaces in bulk-planar and nanowire form. Both periodic "superlattice" geometries and slabs finite along the surface normal are compared. We compute interface atomic and electronic structure, and for small-diameter nanowires, we discuss the impact of quantum confinement, intrinsic strain, and organic ligand passivation on the electronic properties of the interface. Our results are discussed in the context of recent experiments.

[1]Prepared at LBNL under U.S. DOE contract DE-AC02-05CH11231.

Shenyuan Yang
Molecular Foundry, Lawrence Berkeley National Laboratory

Date submitted: 20 Nov 2008 Electronic form version 1.4