Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Models for (001) epitaxial interfaces between CdTe and ZnO[1] JOHN JAFFE, TIFFANY KASPAR, TIMOTHY DROUBAY, Pacific Northwest National Laboratory — Epitaxial interfaces between ZnO and CdTe appear difficult to achieve given their different crystal structures (CdTe is zinc blende with conventional lattice constant a = 6.482 Å, ZnO is hexagonal wurtzite with a = 3.253 Å and c = 5.213 Å.) However, ZnO also occurs in a metastable zinc-blende structure with an fcc primitive lattice constant close to the hexagonal a value. Since this value is close to half of the CdTe conventional (simple cubic) lattice constant, (001)-oriented cubic ZnO films might grow epitaxially on a CdTe (001) surface in an R45° $\sqrt{2}\times\sqrt{2}$ configuration. Many alignments of the interfacial layers are possible, and we describe density-functional calculations on several of these to identify the most likely, and to predict valence-band offsets between CdTe and ZnO for each. Growth of ZnO on Te-terminated CdTe (001) is predicted to produce small or even negative (CdTe below ZnO) valence band offsets, resulting in a Type I band alignment. Growth on Cd-terminated CdTe is predicted to produce large positive offsets for a type II alignment as needed, for example, in solar cells. Calculations with the GGA + U method (with U = 7.5 eV for Zn 3d states) gave a valence band offset of +1.8 eV while a hybrid HSE06 + U calculation gave +2.6 eV. An experimental measurement on a ZnO film grown on CdTe (001) yielded a value of +2.2 eV for the valence band offset.

[1]Supported by PNNL LDRD funding.

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Date submitted: 31 Oct 2011 Electronic form version 1.4