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Calculated Stability and Band Offsets for Compensated and Abrupt Polar Si/Zn(S,Se) (111) Interfaces[1] DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — Heterovalent semiconductor interfaces, particularly in the non-symmetrizable (111) and (0001) directions, present computational challenges that must be addressed in order to predict properties such as band offsets and interface energies. We perform first principles GGA+U calculations of interface energies and band offsets for the nominally polar interfaces Si/Zn(S,Se) (111). Such wide-gap/narrow-gap heterostructures have been proposed as a possible means for altering the relaxation channel branching ratios for the decay of high energy photoelectrons (blue to UV) in favor of impact ionization (two carrier pairs from one photon). Examining configurations with one and two substitutional defect layers, we find the expected trend that compensated interfaces typically have lower energies than abrupt interfaces. The valence band offset (-0.8 ± 0.1 eV) for the lowest energy abrupt Si/ZnS interfaces agrees well with the experimentally determined value of -0.7 eV. We examine methods to address the ambiguities that arise from both finite size induced inter-interface charge transfer and the non-symmetrizability of (111) oriented supercells.

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