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Band alignment and interface charge decomposition for abrupt and polar-compensated Si/ZnS interfaces[1] DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — Using the DFT+U method, we study abrupt and polar-compensated Si/ZnS interfaces in the (100), (110), and (111) directions, examining computational and physical aspects of asymmetric supercells. Distinct interfaces derived from the (100) and (111) directions have valence band offsets (VBO) near either -0.9 eV or -2.1 eV. This bimodal interface dipole distribution is surprisingly obeyed by single-substitution polar-compensated interfaces as well as abrupt polar interfaces. The VBO in the non-polar direction (110) is near the mean value of the distribution (-1.5 eV). Examining one stoichiometric (111) superlattice, we find that the interface free charge, estimated directly from partial occupation of nominally unoccupied surface states, is in good agreement with prediction from the calculated electric fields and dielectric properties. Specifically, the sum of the free charge determined by state occupation, the induced bound charge, and the compositional charge (interface theorem bound charge) is equal to the total interface charge.

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