

Comment on "Heterojunction valence-band-discontinuity dependence on face orientation"

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In a recent Rapid Communication [Phys. Rev. B 35, 6468 (1987)], Muñoz, Sánchez-Dehesa, and Flores presented a self-consistent tight-binding analysis of valence-band offsets in GaAs/AlAs and CdTe/HgTe, and found a sizable dependence upon interface orientation for the latter system. This result differs from that obtained by the present authors for CdTe/HgTe heterojunctions. A more general study, building upon our previous heterojunction calculations, indicates in fact that independence of interface orientation is a general characteristic of a wide class of nonpolar interfaces.

The self-consistent tight-binding method used by Muñoz *et al.*¹ offers a relatively simple way of calculating charges and potentials at semiconductor interfaces. Their values for valence-band discontinuities agree reasonably well with reliable experimental data and with self-consistent local-density-functional calculations by the present authors.^{2,3} When studying the dependence on interface orientation, however, they found a sizable difference between the (110) and (100) orientations for the CdTe/HgTe system, contrary to the result obtained by the present authors for that system. We have in fact studied the dependence on interface orientation in several other cases, and always found it to be negligible. The results presented here are an extension of our full self-consistent interface calculations on a wide variety of lattice-matched and strained-layer interfaces, based on local-density-functional theory and using *ab initio* pseudopotentials. Such calculations take the detailed electronic charge distribution around the interface into account, and thus automatically include all screening effects. The methods and a number of results have been presented before,²⁻⁴ including a discussion of orientation independence of the offsets in GaAs/AlAs. Here we present new results for CdTe/HgTe and AlSb/GaSb interfaces in the (100), (110), and (111) orientations. We will discuss our calculational procedure, show the results for various interfaces, and suggest possible reasons why the tight-binding method of Muñoz *et al.* yields different results.

Interface calculations were performed on supercells containing 8 [for (100)] or 12 [for (110) and (111)] atoms. The wave functions and potentials were expanded in plane waves up to an energy cutoff of 6 Ry. In some cases we tested these results by going up to 9 Ry (corresponding to more than 850 plane waves); since the changes were less than 0.03 eV, we established that our results were converged in terms of the wave-function expansions. However, for the present purposes, the most important point is that we compare calculations for different orientations done with exactly the same cutoff.

The convergence with respect to the number of sampling points in the Brillouin zone is more difficult since we are comparing results calculated with different grids of k points. To establish convergence, we increased the number of special points in a GaAs/AlAs calculation from 3 to 10 in the (100) and (111) orientations, and from 4 to 9 in the (110) orientation. This resulted in changes in the lineups smaller than 0.01 eV, which allows us to be confident that our small k -point sets suffice. The convergence with respect to cell size was checked on the (100) supercells, where increasing the number of atoms from 8 to 12 changed the lineups by less than 0.01 eV (we actually found that even a four-atom supercell can predict a value for the lineups that agrees with the larger calculations to within 0.1 eV).

We use the interface calculations to obtain a value for the potential lineup across the interface; we can then refer the band structures calculated for individual bulk semiconductors to these potentials. Bulk calculations were performed with an energy cutoff of 18 Ry. The pseudopotentials treat the d electrons in Ga, Cd, and Hg as core electrons; including these as valence electrons may have a small effect on the offsets due to hybridization effects, but should have no influence on the comparison between different interface orientations. The overall numerical accuracy of the band discontinuities derived from these calculations is on the order of 0.1 eV; certain systematic errors inherent to the local-density-functional approximation and the use of pseudopotentials are expected to cancel, so that the accuracy of the *difference* between values derived for different interface orientations will be at least as good as this numerical accuracy of 0.1 eV.

In Table I we list our results for valence-band discontinuities. It is clear that for all the lattice-matched cases the discontinuity is independent of orientation, to well within the accuracy of the calculations. Table I also contains values for Si/Ge interfaces. Due to the sizable mismatch between these materials, strains must be present in the layers in order to create a pseudomorphic

TABLE I. Valence-band discontinuities for various heterojunctions in different interface orientations. All values are in eV; a positive value for the lineup A/B indicates that the valence band in B is higher in energy than the valence band in A . The values for Si/Ge are for the *average* valence-band discontinuity $\Delta E_{v,av}$.

Heterojunction	(110)	(100)	(111)
CdTe/HgTe	0.27	0.28	0.28
AlAs/GaAs	0.37	0.37	0.39
AlSb/GaSb	0.38	0.39	0.40
Si/Ge	0.53	0.57	0.51

interface.² These strains lead to splittings of the valence bands which significantly alter the lineups. However, it is meaningful to consider a weighted average of these valence bands, $E_{v,av}$, to which the splittings can be added by using deformation potential theory. The value of the discontinuity $\Delta E_{v,av}$ is sufficient to determine the lineup of the band structures. It turns out that the discontinuity in these weighted averages is virtually independent of the specific strain situation of the interface (variation is less than 0.02 eV; averages are given in Table I); furthermore, the comparison in Table I shows that it is also almost independent of interface orientation. One should bear in mind that this result for strained-layer interfaces applies only to the *average* valence-band discontinuity, and that the offsets in the tops of the valence bands may be strongly orientation and strain dependent.

The independence of the offsets on interface orientation in these widely differing cases, going from II-VI to III-V compounds and even strained-layer elemental semi-

conductors, seems to indicate its validity as a general result for a wide class of interfaces. This result should be restricted to nonpolar interfaces; at polar interfaces, the detailed atomic structure can introduce significant dipoles.⁵ The values obtained by Muñoz *et al.* show overall agreement with our results. Their self-consistent tight-binding approach offers a promising calculation scheme, that has the advantage of greater simplicity than the local-density formalism. However, some accuracy is inevitably lost in the process. Investigations by Klepeis and Harrison⁶ indicate that in tight-binding calculations the charge disturbance around the interface can extend much further than is evident from our pseudopotential calculations, and can even contain oscillations whose magnitude depends on the detailed parameters. If such artificial long-range effects are present in the tight-binding calculations, they could be responsible for the differences between different orientations observed by Muñoz *et al.* Also, the fact that charges and potentials can only assume discrete values at the atomic sites offers less flexibility in finding the minimum-energy electronic structure in the self-consistent tight-binding approach. Small inaccuracies in the charges can lead to dipole shifts that significantly change the lineups. It is possible that these constraints introduce changes on the order of the differences between ΔE_v for different orientations that were found in Ref. 1. In contrast, our self-consistent density-functional calculations include more degrees of freedom for the electrons to relax, and clearly indicate that the band offsets discussed here are independent of interface orientation.

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⁵K. Kunc and R. M. Martin, Phys. Rev. B **24**, 3445 (1981).

⁶W. A. Harrison (private communication).