Comment on "Empirical fit to band discontinuities and barrier heights in III-V alloy systems"

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In a recent letter Tiwari and Frank[1] "present a figure summarizing the variation of ...band discontinuity ... and gold Schottky barrier height for binary and ternary III-V semiconductors." Figures constructed in the same way were presented earlier by McCaldin and co-workers[2–4] for binary compounds, including the III-Vs, and by Schuermeyer *et al.*[5] for ternary III-Vs. As for the numerical values used in the Tiwari and Frank figure, their energy values for binary III-V compounds are in excellent agreement with values presented[6] in 1976, which they seem to be unaware of. Thus yet undiscussed aspects of their letter are (1) the relevance of a previously described graphical presentation and (2) agreement with sixteen year old data.

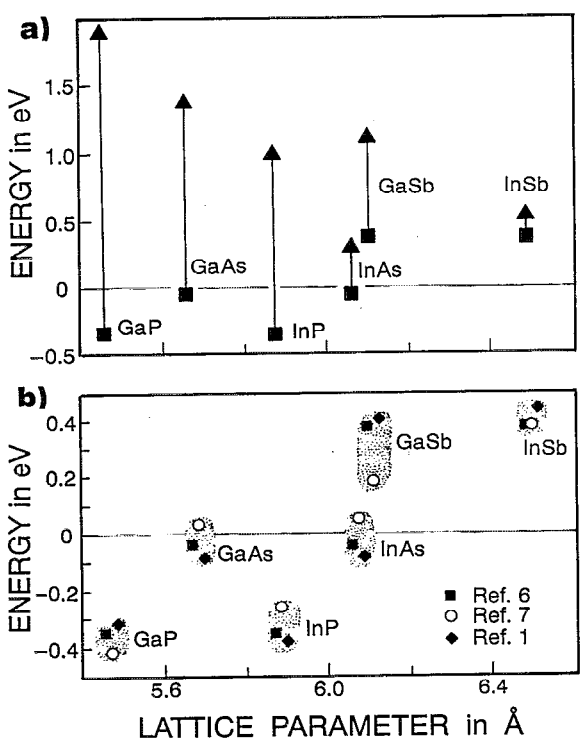

FIG. 1. Energy positions for III-V compounds common to Refs. 1, 6, and 7. This plot follows the format of Refs. 2–4, in which the symbols represent band edge positions and the vertical arrows band gaps E_g. Note that the various E_g are staggered so that band offsets can be read by comparing any two compounds. (a) Valence band edge (filled squares) and conduction band edge (filled arrows) according to Ref. 6. (b) An expanded plot to show predicted valence band positions E_v for Refs. 1, 6, and 7. In (b) the correct lattice parameter occurs at the square symbols and the other two symbols are slightly displaced to the right.

Figure 1 plots energy predictions for those III-V compounds which are common to Refs. 1, 6, and 7, the latter being the often-used values given by Katnani and Margaritondo.[7] Values for valence band edge energy E_v and conduction band edge energy E_c in Fig. 1(a) are those of Ref. 6, however. Unlike the usual plots of energy gap E_g vs lattice parameter, this plot relates all E_v energies to a common zero, so band offsets between any two semiconductors can be read directly from the plot.[2–4] A similar plot appears in Ref. 1, so that one could compare predictions of Refs. 1 and 6 from such plots.

Comparison is facilitated, however, by Fig. 1(b). This plot deals with the difficulty that there is usually no accurate absolute reference energy for such comparisons. Consequently, each of the three sets of E_v predictions plotted in Fig. 1(b) has its arithmetic mean value positioned at a common zero, which minimizes deviations between any two sets and enables calculation of rms deviations.

The excellent agreement between Tiwari and Frank[1] and the unquoted McCaldin, McGill, and Mead[6] paper is apparent in Fig. 1(b), where filled symbols denote these two references. The rms deviation for the six compounds common to these two sets of predictions is only 41 meV. On the other hand, neither of these two references is in such good agreement with Katnani and Margaritondo,[7] which has a rms deviation of 135 meV with Ref. 1 and 105 meV with Ref. 6. A later Margaritondo paper[8] included an AlAs value. This plus Si and Ge values are common to Refs. 1 and 8, enabling a comparison between nine materials. The resulting rms deviation increases, however, to 148 meV. Reference 6 did not include Al pnictides as "...barriers reported on *n*-AlAs and *p*-AlSb do not follow the trends discussed...," the trends referred to being what is now called the "common anion rule". Other author's band edge positions have been analyzed in a similar way in Ref. 3, with rms deviations varying between 105 and 501 meV.

It should be mentioned that one particular comparison can be made on an absolute energy scale, since Refs. 1 and 6 both refer to the Fermi level, E_{fs} in gold. On this basis an arithmetic comparison of the two predictions gives a disagreement of 67 meV.

In summary, we believe that while new presentations like that of Tiwari and Frank[1] are indeed useful, they should include some historical perspective.

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