ERRATA

Erratum: Tetrahedral structures and phase transitions in III-V semiconductors [Phys. Rev. B 50, 8389 (1994)]

J. Crain, R. O. Piltz, G. J. Ackland, S. J. Clark M. C. Payne, V. Milman, J. S. Lin, P. D. Hatton, and Y. H. Nam

We report revised calculations with improved accuracy to those in the 1994 paper which demonstrated the theoretical stability of the SC16 structure in III-V compounds under pressure, and the kinetic barriers to its experimental formation.

In a recent paper by Mujica, Needs, and Munoz,[1] it was claimed that the calculations contained in our original paper for GaAs were not completely converged. We have investigated possible sources of error, and found that for the wurtzite and diamond structures the k-point sampling which we used, while adequate for diamond and lonsdaleite, was insufficient for the compounds.

We have rerun our calculations using grids of $9\times9\times9$ k points for the zinc-blende structure with two atoms, reduced by symmetry to 35 nonequivalent k points. For the wurtzite structure, a grid of $7\times7\times4$ k points for the larger four-atom cell was used. At this sampling density the energy is converged with respect to k-point density to within 0.002 eV/atom, as compared with single runs of the ground-state structure with even finer grids. For the SC16 the k-point sampling was thoroughly described in the previous paper, and is accurate. The result for GaAs is in good agreement with that found by Mujica, Needs, and Munoz, and our wurtzite–zinc-blende differences are now in agreement with the work of Yeh *et al.*[2]

Moreover, the difference between the c/a ratios and the ideal value is very dependent on k-point sampling. Contrary to what we said in our previous paper, stable wurtzite structure c/a ratios are *smaller* than ideal (GaAs $c/a=1.6499$, InAs $c/a=1.6354$, and for AlSb $c/a=1.6442$). The energy differences between wurtzite and diamond are also much smaller, of order 0.01 eV/atom.

The revised figures for the pressure-volume relations are shown in Fig. 1. Also, the value of V_0 for BC8-GaAs should be 18.86 Å^3.

The sequence of phase stability is unchanged, and the main conclusions of our paper (that SC16 has a range of thermodynamic stability in all compounds) are also unchanged. However, the pressure range of this stability is reduced with predicted transition pressures from diamond to SC16 being increased to 109 kbar (GaAs), 66 kbar (InAs), and 46 kbar (AlSb).

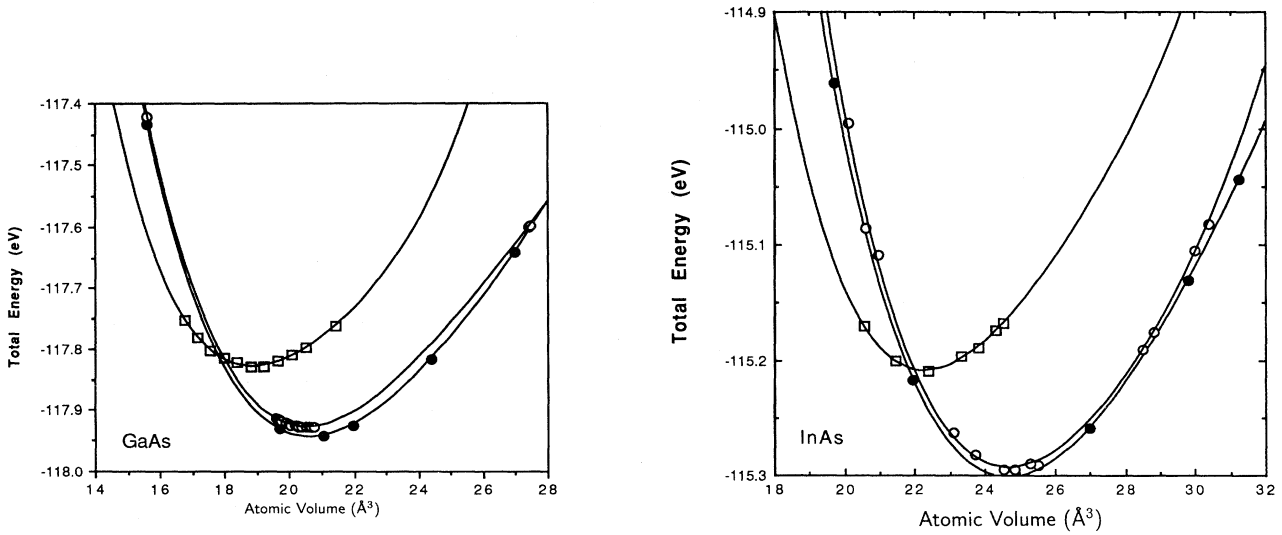

FIG. 1. Total energy vs atomic volume for (a) GaAs, (b) InAs, and (c) AlSb in the diamond (filled circles), wurtzite (open circles), and SC16 (squares) structures. The lines are polynomial fits to the data.

0163-1829/95/52(23)/16936(2)/$06.00

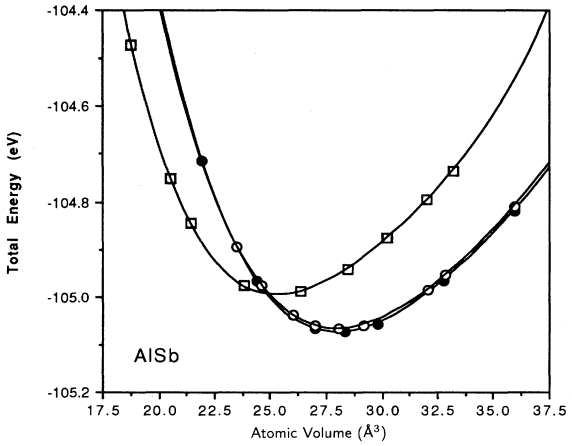

FIG. 1. (*Continued*).

Since our prediction of this structure, x-ray diffraction peaks consistent with SC16, though not identified as such, have been reported in depressurized GaAs in the range 5–10 GPa.[3]

[1]A. Mujica, R. J. Needs, and A. Munoz, Phys. Rev. B **52**, 8881 (1995).
[2]C. Y. Yeh, Z. W. Lu, S. Froyen, and A. Zunger, Phys. Rev. B **46**, 10086 (1992).
[3]K. Tsuji, Y. Katayama, Y. Yamamoto, H. Kanda, and H. Nosaka, J. Phys. Chem. Solids **56**, 559 (1995).

Erratum: Exact solutions for barrier D^- states at high magnetic fields [Phys. Rev. B 51, 10 709 (1995)]

Herbert L. Fox and David M. Larsen

We have found an error in our calculation of the symmetric $M=-4$ state, which tends to produce too small binding for that state. The correct binding is presented in Fig. 1 below, which replaces Fig. 3 of the original article.

This revision requires that the description of the sequence of ground states appearing in the abstract and in the last paragraph of the first column of p. 10711 be changed. The correct sequence of ground-state wave functions for the barrier D^- center is $M=0$ singlet$\rightarrow M=-1$ triplet$\rightarrow M=-2$ singlet$\rightarrow M=-3$ triplet$\rightarrow M=-4$ singlet$\rightarrow M=-5$ triplet as α increases from zero. Also, the first range of α for which eight bound states coexist, originally given as "between 0.41 and 0.48," should be changed to "between 0.46 and 0.48."