Comment on "Predicted Modifications in the Direct and Indirect Gaps of Tetrahedral Semiconductors"

In a recent Letter,[1] Rompa, Schuurmans, and Williams used the augmented spherical-wave (ASW) method to compute the electronic charge density of GaAs at the Γ and X k points of the first conduction band. They observed a striking difference between the charge densities at these two points and suggested that while self-consistent pseudopotential calculations with a plane-wave basis might be able to confirm this, tight-binding calculations with on-site s, p, and d functions would not.

We wish to point out in this Comment that although first-principles calculations have not been used to explore this problem, this observation has been made previously for Ge[2] and other III-V semiconductors[3] using the empirical pseudopotential method (EPM); and that *both* the EPM scheme, which uses an *extended* plane-wave basis, and the linear combination of atomiclike orbitals (LCAO) approach,[4] which employs an *on-site* Gaussian orbital basis, are capable of computing charge densities at selected k points in the Brillouin zone of a given semiconductor.

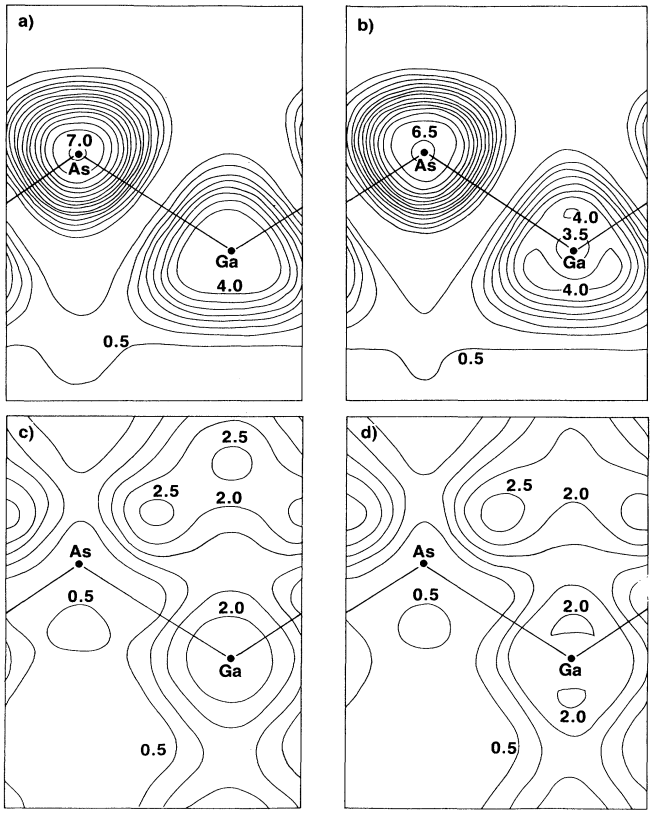

FIG. 1. Contour plots of the electron charge density of the first conduction band in GaAs in the $(1\bar{1}0)$ plane: (a) at Γ (EPM); (b) at Γ (LCAO); (c) at X (EPM); and (d) at X (LCAO). The contour interval is 0.5 in units of electron per primitive cell.

We construct a model potential for GaAs and use it to calculate the band structure and charge densities of GaAs using both approaches.[5] The eigenvalues obtained by both methods agree to within 0.1 eV for the first conduction band, and the computed charge densities at the Γ and X points are shown in Fig. 1. The charge density at Γ is characterized by antibonding s-like orbitals on the Ga and As ions while the X state has a more uniform charge density since it involves mostly antibonding d and p orbitals. The enhanced charge density in the interstitial region at X is also evident.

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