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Review

Electronic structure modeling of InAs/GaSb superlattices with hybrid density functional theory

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HIGHLIGHTS

- Superlattice band gap data using density functional theory is presented.
- A PBE0-type hybrid functional was used.
- Our approach requires only experimental measurements of the constituent materials' band gaps.

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ABSTRACT

The application of first-principles calculations holds promise for greatly improving our understanding of semiconductor superlattices. Developing a procedure to accurately predict band gaps using hybrid density functional theory lays the groundwork for future studies investigating more nuanced properties of these structures. Our approach allows a priori prediction of the properties of SLS structures using only the band gaps of the constituent materials. Furthermore, it should enable direct investigation of the effects of interface structure, e.g., intermixing or ordering at the interface, on SLS properties. In this paper, we present band gap data for various InAs/GaSb type-II superlattice structures calculated using the generalized Kohn-Sham formulation of density functional theory. A PBE0-type hybrid functional was used, and the portion of the exact exchange was tuned to fit the band gaps of the binary compounds InAs and GaSb with the best agreement to bulk experimental values obtained with 18% of the exact exchange. The heterostructures considered in this study are 6 monolayer (ML) InAs/6 ML GaSb, 8 ML InAs/8 ML GaSb and 10 ML InAs/10 ML GaSb with deviations from the experimental band gaps ranging from 3% to 11%.

InAs/GaSb type-II strained layer superlattices (SLS) have attracted considerable research interest for use as mid-and long-wavelength infrared photodetectors [1]. The absorption wavelength of these superlattices can be tuned between 3 μm and 32 μm, depending on the thicknesses of the constituent InAs and GaSb layers [2–4]. High quality InAs/GaSb SLS can be grown experimentally due to their low lattice mismatch [5]. InAs/GaSb SLS also exhibit comparable quantum efficiency and lower Auger current than bulk HgCdTe detectors of comparable band gap [6–8].

A superlattice is a periodic structure of two or more crystalline materials, typically semiconductors with differing band gaps, the layers of which tend to be on the order of several nanometers. This technique modifies the energies and wave functions of the near-band-gap electronic states leading to novel optical and transport properties. The current standard for classifying superlattices is to group them by their confinement energy schemes. Type-II superlattices are composed of spatially indirect band gap semiconductors which confines the electrons and holes in different layers. Theoretically the extreme type-II energy alignment of an InAs/GaSb SLS allows one to achieve any desirable long wave IR band gap for IR detection by tuning their effective band gap.

In an InAs/GaSb SLS, the electron and hole wave functions are partially confined within the InAs and GaSb layers respectively as seen in Fig. 1. Due to this partial confinement, carrier energies are increased relative to carriers in the relevant bulk materials, i.e., the lowest unoccupied (electron) states of the SLS are higher in energy than the conduction band minimum of InAs, and the highest occupied (hole) states of the SLS are lower in energy than the valence band maximum of GaSb. Since the hole states in GaSb are higher in energy than the electron states in InAs, InAs/GaSb SLS

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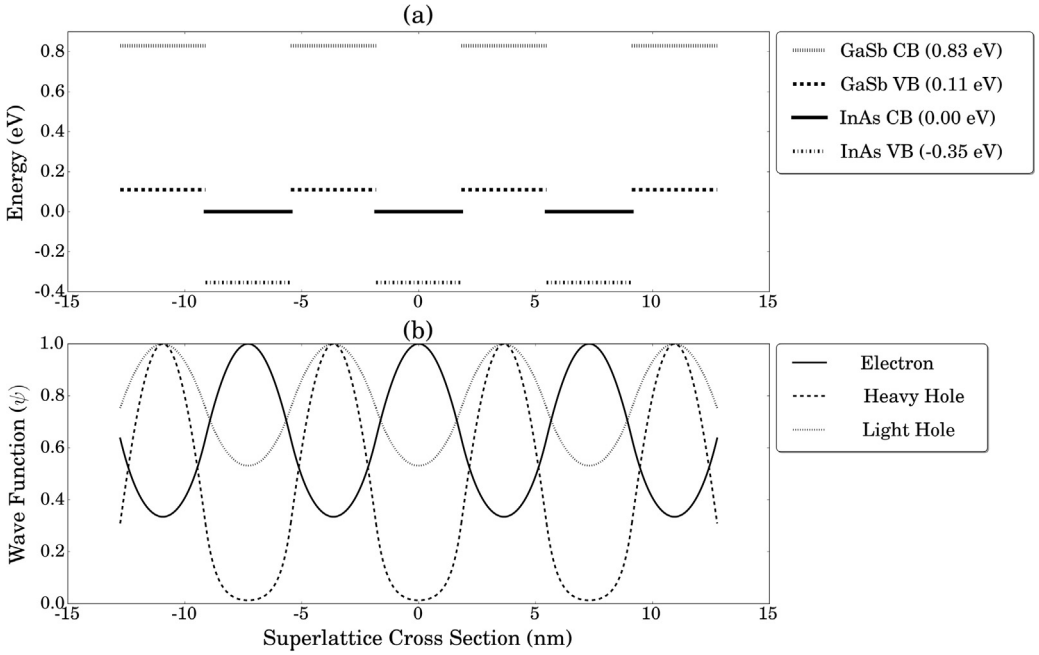

Fig. 1. (a) Shows type-II band alignment of the conduction bands (CB) and valence bands (VB) of an InAs/GaSb type-II SLS. (b) Shows low-energy electron and hole envelope functions obtained from a simple one-band effective mass model for an InAs/GaSb type-II SLS.

can be tuned, in principle, from metallic behavior through a range of long wave IR band gaps by varying the thickness of the constituent layers, and thus the extent of confinement. Due to tunneling through the intervening barrier layers (i.e., GaSb for electrons and InAs for holes), these partially confined states form bands with a small dispersion in the SLS stacking direction, which are called minibands. In the valence band, confinement has less of an effect on the heavy hole (HH) states than on the light hole (LH) states, and the HH derived minibands are higher in energy than the LH minibands. Therefore, photons are detected in an InAs/GaSb SLS by inter-subband transitions between the highest HH miniband and the lowest electron miniband [9], and the difference between the energies of these minibands defines the band gap of the SLS.

The $\mathbf{k}\cdot\mathbf{p}$ theory has been successfully used to calculate accurate band gaps for InAs/GaSb SL [15–17,20]. However, the band gaps of SLS structures depend on a large number of parameters in addition to the band gaps of the constituent materials, including band masses, band offsets, and interface properties, as well as the strain dependence of these quantities. The development of accurate empirical models for the properties of SLS structures requires sufficient experimental input such as valence and conduction energy levels, spin-orbit energy, electron effective mass, lattice constants, elastic constants, deformation potentials, and Luttinger parameters. In addition, the $\mathbf{k}\cdot\mathbf{p}$ theory is a continuum theory that lacks a representation for specific atoms, and therefore, there is no straightforward approach to predict properties such as point defects for which the local atomistic structure differs significantly from the host crystal. The non-trivial interface effect seen in a InAs/GaSb SLS is also not accounted for using conventional $\mathbf{k}\cdot\mathbf{p}$ theory, although to mitigate these interfacial and symmetry-breaking effects some additional terms could be introduced [18,19].

Despite their record of success in a variety of semiconductors, conventional Density Functional Theory (DFT) functionals, based on the local density and generalized gradient approximations (LDA and GGA), generally give vanishing band gaps for InAs, GaSb [10], and, as we report in this work, InAs/GaSb superlattices. In contrast, hybrid functionals, e.g., PBE0, B3LYP, and HSE06, have been shown to give more accurate band gaps for bulk semiconductors, including narrow band gap semiconductors such as InAs and GaSb [11–13]. Accurate calculations for the band gaps of InAs/GaSb SLS, where the superlattice minibands are only separated by a few tenths of an eV, can be expected to be even more challenging. In addition to bulk band gaps, accurate calculations of SLS band gaps require an accurate treatment of a number of other properties of the constituent materials such as band masses and band offsets. Thus, an accurate first principles approach to calculating the properties of SLS structures would be invaluable.

In this letter, we investigate the accuracy of InAs/GaSb superlattice band gap calculations using hybrid DFT functionals. We are building upon the previous work of Wang et al. who, using the LDA, was able to calculate accurate SLS band gaps by applying an empirical method to correct bulk band gaps [14]. We will first report the technical parameters used in the bulk and superlattice hybrid DFT calculations performed for this study. We then will discuss our band-gap and lattice constant results for bulk InAs and GaSb and our procedure for optimizing the mixing factor used in our PBE0-like functional. Next, we will describe our procedure for performing hybrid superlattice calculations, which will be followed by our calculated results for the band gaps of three InAs/GaSb SLS and discussion of these results.

Our hybrid DFT calculations were performed using the open-source Socorro DFT package [22]. A plane wave basis with a 40 Rydberg cutoff was used to represent the valence Kohn Sham orbitals, and norm conserving pseudopotentials (NCPs) were used to represent the effect of the nuclei and atomic cores on the valence electrons. The NCPs were constructed for the PBE exchange-correlation functional using the fhi98PP [23] code with three electrons treated as valence (ns^2 and np^1) for Ga ($n = 4$) and In ($n = 5$), and five electrons treated as valence (ns^2 and np^3) for As ($n = 4$) and Sb ($n = 5$). We were unsuccessful in our attempts to construct an In pseudopotential without ghost states using the fhi98PP code, and the In pseudopotential used in our calculations was obtained from the Abinit website [24]. Monkhorst-Pack [25] k-point meshes shifted to include the Γ point were used to sample the Brillouin zone with a $8 \times 8 \times 8$ mesh used for bulk unit cells and a $4 \times 4 \times 1$ mesh used for the SLS structures. While the bulk