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NARROW GAP III-V SEMICONDUCTORS : ELECTRONIC AND STRUCTURAL PROPERTIES

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Abstract: The structural and electronic properties of narrow gap InX (X=P, As, and Sb) are studied with first-principle schemes by using both the full-potential linearized augmented plane wave method and norm-conserving pseudopotentials. Our results compare favourably with the available experiment.

Studies of the electronic and structural properties of binary semiconductors have recently received considerable attention, both experimentally and theoretically. However, despite interesting properties related to their narrow energy gaps, the InX compounds (X = P, As, and Sb) [1] have barely been studied in comparison to the extensive work performed on other zincblende materials like GaAs, AlAs and ZnSe. Furthermore, the recently achieved epitaxial growth of InAs/InP superlattices [2] has provided good single crystals suitable for accurate experimental measurements and has added new interest to the study of the constituent bulk semiconductors.

In this work, intended as a first step towards a detailed study of their superlattice compounds, we investigate the structural and electronic properties of these semiconductors. We use the full-potential linearized augmented plane wave (FLAPW) [3] and the ab-initio norm-conserving pseudopotential (PS) methods [4] to investigate the electronic and structural properties of InP, InAs, and InSb in their zincblende structure. The study indicates the importance of the "semicore" In 4d states, which play a role in the electronic structure of these materials similar to that of the Ga 3d states in GaAs, and the cation d states in the zincblende II-VI compounds [5,6,7,8]. Furthermore, this study shows that, within the local density approximation (LDA), InAs and InSb have metallic properties. This fact may be intended as a result of the well-known failure of LDA in the description of the excitation properties of semiconductors. By contrast, the pressure dependence of energy gaps compares favorably with the

existing experiment. On the other hand, excellent agreement is found with experiment for the equilibrium properties of these materials and an agreement within the experimental resolution is found for the occupied energy bands.

The equilibrium properties, i.e. lattice constants, bulk moduli and their derivatives, are in excellent agreement with the experimental results [9] when calculated with the FLAPW method. The smaller lattice parameters, understimated of about 2%, obtained with the pseudopotential approach emphasizes the role of the shallow In 4d semi core states in determining the structural properties of these compounds.This may be attributed to the contribution of the In 4d states which is neglected in the PS approach, since similar differences between all-electron and PS results were found in GaAs and ZnSe [10,11]. Similar results have been obtained for II-VI materials [8] and for ternary zincblende defective compounds [12].

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