

Zeitschrift: Helvetica Physica Acta

Band: 62 (1989)

Heft: 6-7

Artikel: Narrow gap III-V semiconductors : electronic and structural properties

Autor: Pascale, T.M. de / Meloni, F. / Serra, M.

DOI: <https://doi.org/10.5169/seals-116132>

Nutzungsbedingungen

Die ETH-Bibliothek ist die Anbieterin der digitalisierten Zeitschriften auf E-Periodica. Sie besitzt keine Urheberrechte an den Zeitschriften und ist nicht verantwortlich für deren Inhalte. Die Rechte liegen in der Regel bei den Herausgebern beziehungsweise den externen Rechteinhabern. Das Veröffentlichen von Bildern in Print- und Online-Publikationen sowie auf Social Media-Kanälen oder Webseiten ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. [Mehr erfahren](#)

Conditions d'utilisation

L'ETH Library est le fournisseur des revues numérisées. Elle ne détient aucun droit d'auteur sur les revues et n'est pas responsable de leur contenu. En règle générale, les droits sont détenus par les éditeurs ou les détenteurs de droits externes. La reproduction d'images dans des publications imprimées ou en ligne ainsi que sur des canaux de médias sociaux ou des sites web n'est autorisée qu'avec l'accord préalable des détenteurs des droits. [En savoir plus](#)

Terms of use

The ETH Library is the provider of the digitised journals. It does not own any copyrights to the journals and is not responsible for their content. The rights usually lie with the publishers or the external rights holders. Publishing images in print and online publications, as well as on social media channels or websites, is only permitted with the prior consent of the rights holders. [Find out more](#)

Download PDF: 21.02.2026

ETH-Bibliothek Zürich, E-Periodica, <https://www.e-periodica.ch>

NARROW GAP III-V SEMICONDUCTORS : ELECTRONIC AND STRUCTURAL PROPERTIES

T.M. de Pascale and F. Meloni

Dipartimento di Scienze Fisiche, Universita', 09124 Cagliari, Italy

M. Serra

Istituto di Fisica Superiore, Universita', 09124 Cagliari, Italy

S. Massidda, A. Continenza and A.J. Freeman

Material Research Center and Department of Physics and Astronomy
Northwestern University, Evanston, Illinois, 60208

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, underestimated 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].

Work (at Northwestern University) was supported by the National Science Foundation (through the Northwestern University Materials Research Center Grant No. DMR88-21571) and by a computing grant from its Division of Advanced Scientific Computing at the National Center for Supercomputing Applications, University of Illinois, Champaign/Urbana.

References

- [1] *Proceedings of the 4th International Conference on Physics of Narrow Gap Semiconductors*, Edited by E. Gornik, H. Heinrich and L. Palmetshofer (Springer-Verlag, 1982).
- [2] R.P. Schneider, D.X. Li and B.W. Wessel in "*Heteroepitaxial Approaches in Semiconductors: Lattice Mismatch and Its Consequences*", ed. A.T. Macrander Electrochemical Soc. Pennington (NJ)(in press); R.P. Schneider, D.X. Li and B.W. Wessels, *Electr. Chem. Soc.* (in press); D.V. Lang, M.B. Panish, F. Capasso, J. Allam, R.A. Hamm, A.M. Sergent and W.T. Tsang, *J. Vac. Sci. Technol.* **B5**, 1215 (1987).
- [3] H.J.F. Jansen and A.J. Freeman, *Phys. Rev.* **B30**, 561 (1984).
- [4] G.B. Bachelet, D.R. Hamann, and M. Schlüter, *Phys. Rev.* **B26**, 4199 (1982).
- [5] G.B. Bachelet and N.E. Christensen, *Phys. Rev.* **B31**, 874 (1985).
- [6] N.E. Christensen, *Phys. Rev.* **B37**, 4528 (1988).
- [7] S.H. Wei and A. Zunger, *Phys. Rev. Lett.* **59**, 144 (1987).
- [8] S.H. Wei and A. Zunger, *Phys. Rev.* **B37**, 8958 (1988).
- [9] *American Institute of Physics Handbook* (McGraw-Hill, New York, 1987).
- [10] B.I. Min, S. Massidda and A.J. Freeman, *Phys. Rev.* **B38**, 1970 (1988).
- [11] A. Continenza, S. Massidda and A.J. Freeman, *Phys. Rev.* **B38**, 12996 (1988).
- [12] J.E. Bernard and A. Zunger, *Phys. Rev.* **B36**, 3199 (1987).