

Energy Band Structure of InAs with MedeA[®]-VASP

The energy band structure of InAs is computed with the HSE06 hybrid functional using MedeA[®]-VASP. The calculations give a direct band gap of 0.35 eV, which coincides with the experimental value. The Γ -L separation in the lowest conduction band is computed to be 1.11 eV. Screened-exchange FLAPW calculations reported a value of 1.21 eV. The earlier handbook value was 0.74 eV. More recent experiments reported 1.1 ± 0.05 eV, which is perfectly consistent with the present calculations.

Keywords: Energy band structure, Γ -L separation, III-V semiconductors, InAs, hybrid functionals, MedeA[®], VASP

Purpose

This application note illustrates the capability of the MedeA[®] software environment with the Vienna Ab initio Simulation Package (VASP) version 5.2 to compute detailed features of the energy band structures of solids such as III-V semiconductors as needed for band structure engineering in electronic and optical devices.

Crystal Structure

The unit cell of InAs is retrieved from the databases available within MedeA[®]. This III-V semiconductor crystallizes in the cubic zincblende structure with lattice parameters reported between 6.0584 Å and 6.060 Å. In the present simulations, a value of 6.0588 Å is used as given by Thompson *et al.* [1]. This allows a direct comparison with previous calculations [2]. A structural optimization using the PBEsol exchange-correlation functional [3] gives a lattice parameter, which is only 0.6% larger than the experimental result.

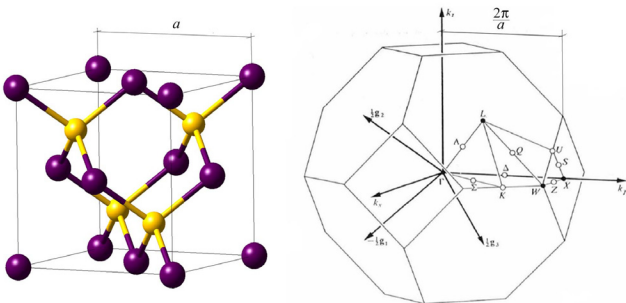


Figure 1. Crystal structure of InAs with the characteristic tetrahedral coordination of both In and As atoms. The drawing on the right hand side shows the corresponding first Brillouin zone with the high-symmetry points and lines labeled according to standard notation.

Band Structure Calculation

The energy band structure is computed with VASP 5.2 as integrated in the MedeA[®] software environment using the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional [4] with the MedeA[®] default parameters for the plane wave cutoff and \mathbf{k} -meshes. The semi-local part is treated on the level of the PBEsol functional [3]. The number of \mathbf{k} -points along the symmetry lines for the band structure is set to 160. The result is shown in Fig. 2.

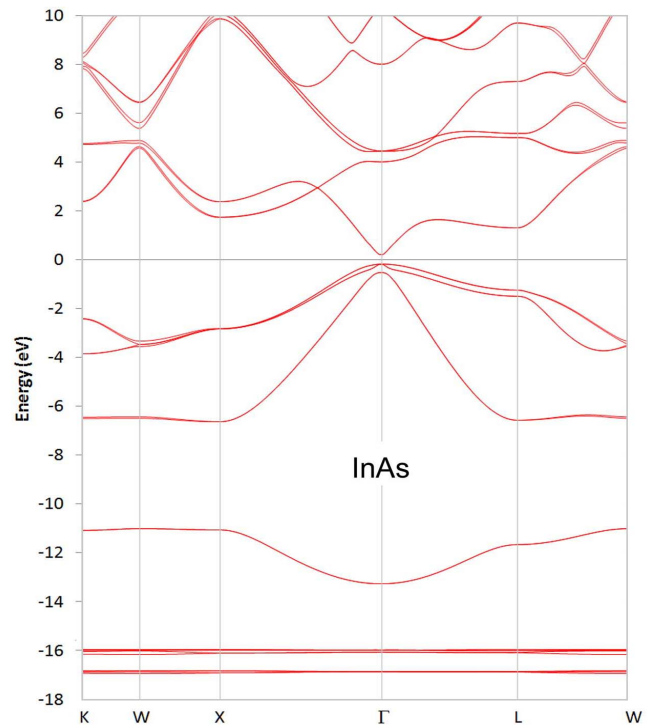


Figure 2. Energy band structure of InAs computed with HSE06 hybrid functional and a spin-orbit relativistic Hamiltonian.

The flat bands between -17 eV and -16 eV are formed by the localized In $4d^{3/2}$ and $4d^{5/2}$ semi-core states, all higher lying bands result from overlap of the s and p states of both atom types. A detailed view of the region near the energy band gap together with a comparison with experimental data is shown in Fig. 3. The agreement between the computed and the experimental direct band gap of $E_g = 0.35$ eV is excellent. Also the computed and measured spin-orbit splitting, E_{so} , at Γ is in quite good agreement.

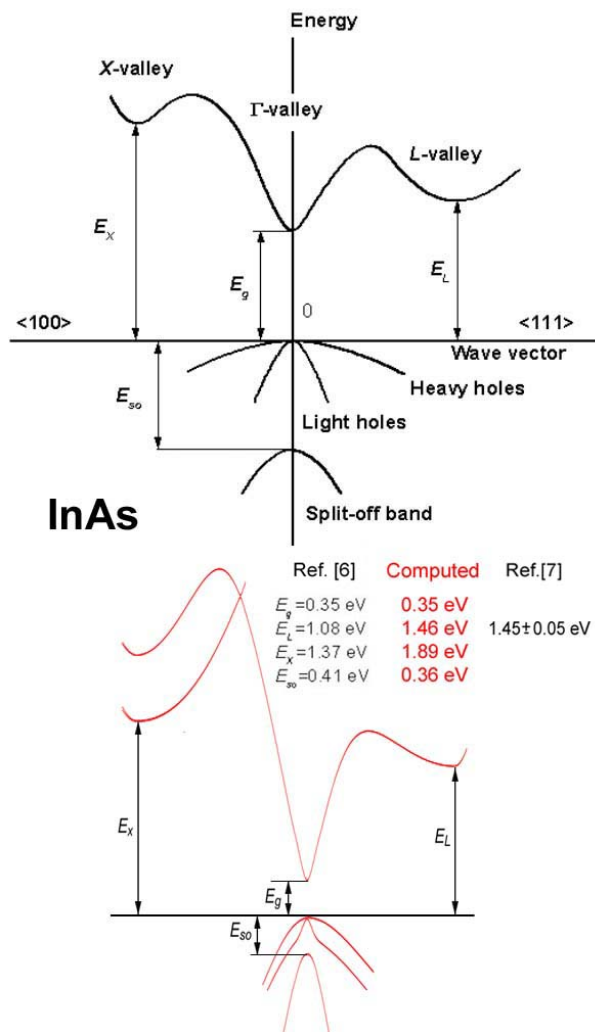


Figure 3. Details of the energy band structure near the energy gap. Note the significant deviations in the position of the X and L-valley comparing the data published on the website of the Ioffe Institute [6] and the computed data and more recent measurements [7].

In contrast, the positions of the X- and L-valleys as reported in Ref. [6] are in marked disagreement with the computed data. In fact, the earlier handbook value of the Γ -L separation, *i.e.* the energy difference

between the bottom of the conduction band and the minimum at the L-point, E_L , has been reported as 0.74 eV [5], which is very close to the value given by the Ioffe Institute [6], namely, $E_L - E_g = 1.08$ eV - 0.35 eV = 0.73 eV (see upper part of Fig. 3). The present calculation gives $E_L - E_g = 1.46$ eV - 0.35 eV = 1.11 eV. Previous calculations using the FLAPW method with screened exchange gave a Γ -L separation of 1.21 eV [2], which is close to the present result. Interestingly, from refined experiments Charache *et al.* obtain a value of 1.1 ± 0.05 eV [7], which is in perfect agreement with the present calculations.

To conclude, while two independent calculations using different computational methods and different many-body exchange-correlation treatments as well as more recent experimental data give values for the Γ -L separation between 1.1 eV and 1.2 eV, the substantial deviation of the earlier value of 0.74 eV casts doubt on the validity of this small value reported in the handbook and also by the Ioffe Institute. Consequently, the computed value for the Γ -X separation is also probably more reliable than the data shown in Fig. 3 from the Ioffe Institute.

Significance

The present case of the energy band structure and position of the L-valley of the conduction band in InAs illustrates that accurate *ab initio* electronic structure calculations can provide quantitative materials property data at a level of accuracy and reliability, which is comparable with experiment. The calculations are systematic as they are free of any atom-specific parameters. This gives the calculations a high predictive power. Furthermore, these types of *ab initio* calculations can be applied to systems under mechanical stress, to alloys, and to surfaces and interfaces, thus allowing the generation of critical parameters for device materials, which may be otherwise difficult, time consuming, or costly to obtain.

MedeA[®] Modules Employed in this Case

The present calculations were performed with the MedeA[®] platform using the following integrated features and modules:

- The standard MedeA[®] framework including crystal structure builders and geometric analysis tools
- MedeA[®]-VASP 5.2 with its graphical user interface
- The MedeA[®] JobServer and TaskServers

- The standard MedeA[®] visualization tools
- The standard MedeA[®] tools for analyzing band structures

References

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