materials design

APPLICATION NOTE

Energy band structure of germanium

Elemental germanium is a semiconductor with a measured indirect band gap of 0.66 eV. Using a hybrid functional as implemented in VASP 5.2, the computed value is 0.66 eV while standard density functional approaches incorrectly predict Ge to have no band gap. Other features of the band structure such as the direct gap at Γ are also well reproduced by the current level of theory, namely 0.8 eV (measured) and 0.73 eV (computed), thus demonstrating the reliability of this level of approach in predicting energy band structures. This sets the stage for using computations to modify the band structure for example by uniaxial strain to meet specific design criteria.

Keywords: energy band structure, band gaps, germanium, computations, hybrid functionals

Experimental facts

Elemental germanium crystallizes in the diamond lattice like silicon. Ge is a prototypical semiconductor with an experimentally determined indirect band gap of 0.66 eV [1], which is the energy difference between the minimum of the conduction band at point L in the Brillouin zone and the top of the valence band at Γ. The direct band gap at the center of the Brillouin zone is measured to be 0.8 eV. Relativistic effects are noticeable. For example the spin-orbit splitting at the Γ point at the top of the valence band is 0.29 eV.

Computed results

The computed energy band structure of Ge using a so-called hybrid functional [2] provides an excellent description of all the major features of the energy band structure as illustrated in Fig. 1. In the present calculation the indirect band gap is computed to be 0.66 eV, which is identical to the experimental value given by the Ioffe Institute [1]. This perfect agreement is probably a coincidence, since the experiments are at room temperature and the calculations correspond to T=0 K. Other features of the band structure such as the direct band gap at the zone center, $E_{\Gamma 1}$, and the minimum energy difference in the direction <100>, ΔE, are reproduced by the calculations with a deviation of less than 0.1 eV. The calculation provide an excellent description of the spin-orbit splitting, E_{so}, of 0.29 eV. This demonstrates that relativistic effects are very well captured at this level of electronic structure calculations.

Significance

The understanding and accurate description of energy band structures is fundamental in the development of electronic devices. Once the accuracy of a computational method is established for a pure system such as demonstrated here for Ge, one can expect the same level of reliability when these materials are subject to stress or shaped as nanostructures, where experimental data might be missing or are difficult to measure. This sets the stage for using computations to achieve specific materials properties, for example by applying a certain uniaxial strain or by confining the dimensions of the system by creating nanostructures.

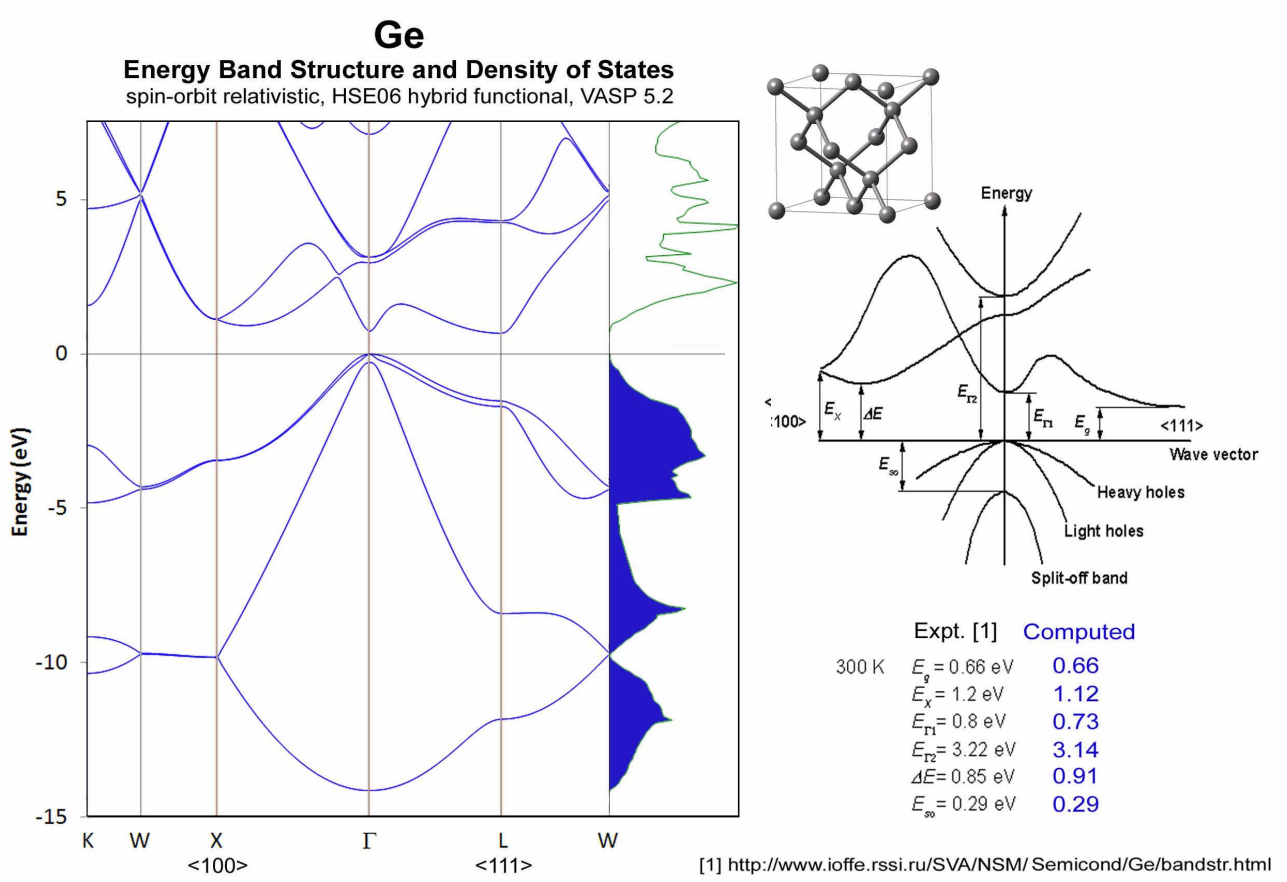

Figure 1. Energy band structure and density of states of elemental germanium as compared with experimental data.

MedeA modules used for this application

The present calculations were performed with the MedeA platform using the following integrated modules of the MedeA software environment

- Standard MedeA framework including crystal structure builders and geometric analysis tools as well as JobServer and TaskServers
- VASP 5.2 and its graphical user interface as integrated in MedeA

Comments

The equilibrium lattice parameter of elemental Ge is very well described (within 0.5% of experiment) by the PBEsol [3] functional, which belongs to the class of semi-local generalized gradient approximations (GGA). Computations with this type of functionals are about two orders of magnitude faster than the hybrid functionals such as the HSE06 functional [2]. In fact the latter is needed for the quantitative description of excitation energies such as band gaps once the geometry of the system is settled.

References

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For further information please contact

Materials Design, Inc.
PO Box 2000,
3465 Mountain View Blvd. #17
Angel Fire, NM 87710, USA
T +1 760 495-4924
F +1 760 897-2179
info@materialsdesign.com
www.materialsdesign.com