# MedeA-VASP 5.2

VASP 5.2, which was released in mid 2009, represents a breakthrough in the calculation of electronic and optical properties for semiconductors and insulators of industrial importance. This is based on an efficient implementation of hybrid functionals and the GW methods. Furthermore, VASP 5.2 offers linear response calculations of properties such as Born effective charges and piezoelectric tensors. The program is fully integrated in the MedeA platform with a graphical user interface enabling the computation of the following properties:

Properties from VASP 5.2

- Total electronic energy of any 3D periodic arrangement of atoms
- Forces on atoms
- Pressure and stress tensors
- Total magnetic moment
- Equilibrium lattice parameters and atomic positions as obtained from energy minimization
- Energy band structure; accurate band gaps, dopant levels, and band offsets based on hybrid functionals and GW methods
- Total and partial (atom and orbital momentum projected) electronic density of states
- Electronic charge density and corresponding electrostatic potentials
- Work functions
- Spin densities
- Magnetic moments
- Response functions including piezoelectric tensors
- Born effective charges
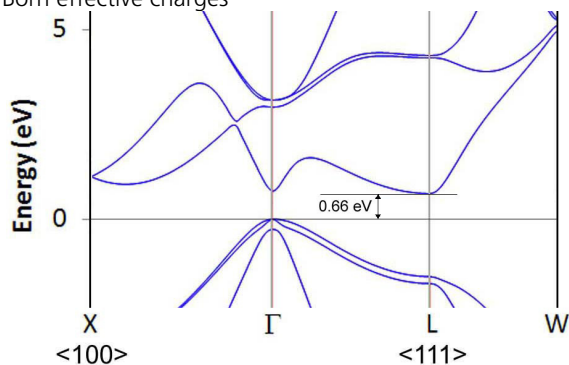
Band gap of germanium correctly predicted with VASP 5.2

- Optical spectra, i.e. dielectric functions, refractive index and optical absorption as a function of frequency

Computational characteristics

- Plane-wave based electronic structure method for periodic structures
- All-electron method with projector augmented wave (PAW) potentials
- Density functional theory (DFT) with local (LDA) and gradient-corrected (GGA) semi-local functionals
- Hybrid functionals; screened exchange, Hartree-Fock
- GW
- Linear response

Other required MedeA modules

- Core MedeA environment
- VASP graphical user interface
- Job Server and Task Servers

More on our website: www.materialsdesign.com

- Adsorption and Dissociation of Iodine Molecules on a Zr Surface
- Energy band structure of germanium
- Ferroelectric Properties of BaTiO₃

Relevant Publications

- J Hafner, *Journal of Computational Chemistry*, vol. 29, no. 13, p. 2044-2078, 2008.
- M Marsman, J Paier, A Stroppa, and G Kresse, *Journal of Physics: Condensed Matter*, vol. 20, p. 064201, 2008
- J Paier, M Marsman, and G Kresse, *Physical Review B Condensed Matter*, vol. 78, p. 121201, 2008.