



materials design

MedeA® VASP 5.2

VASP 5.2, first 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:

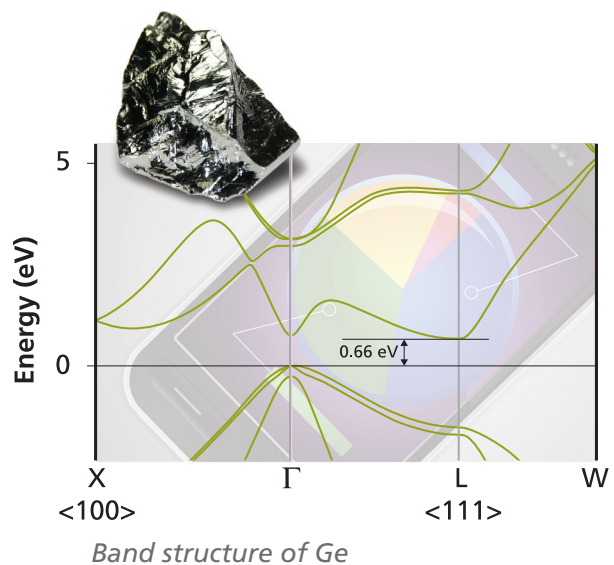
- Total electronic energy of any 3D periodic arrangement of atoms
- Forces on atoms
- Pressure and stress tensors
- Total magnetic moment
- Equilibrium lattice parameters and atomic positions as obtained from energy minimization
- Energy band structure; accurate band gaps, dopant levels, and band offsets 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
- Optical spectra, i.e. dielectric functions, refractive index and optical absorption as a function of frequency

Required MedeA® modules:

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

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: LDA, AM05, PBEsol, PBE, rPBE, BLYP
- Hybrid functionals: HSE06, PBE0, B3LYP
- Screened exchange, Hartree-Fock
- GW method
- Linear response
- D2/Grimme correction for van-der-Waals interaction





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Full Integration

Hybrid calculations can be very time consuming. MedeA® intelligently expands the convergence region so as to minimize the computational time. Combining the DFT and hybrid calculations in one job creates optimized starting conditions and faster convergence for the hybrid component.

The JobServer/TaskServer architecture allows for efficient storage and deployment of temporary files and lets you focus on the science. MedeA® takes care in a transparent way of the important computational details like matching k -meshes and setting adequate VASP parameters.

Tested and Evaluated

With all the combinations of new compilation options it is paramount to ensure that your calculations do not produce erroneous results due to overambitious optimization settings or incorrect compiler flags. Our VASP executables are thoroughly tested in house and our growing family of customers deploy them for an expanding range of applications.

The set of Windows and Linux executables allows the mix and match of architectures, you can run more time consuming calculations and bigger systems on Linux clusters, confident that the results will be consistent with calculations executed on your laptop. No need to redo calculations just to get comparable energies.

More on our website:

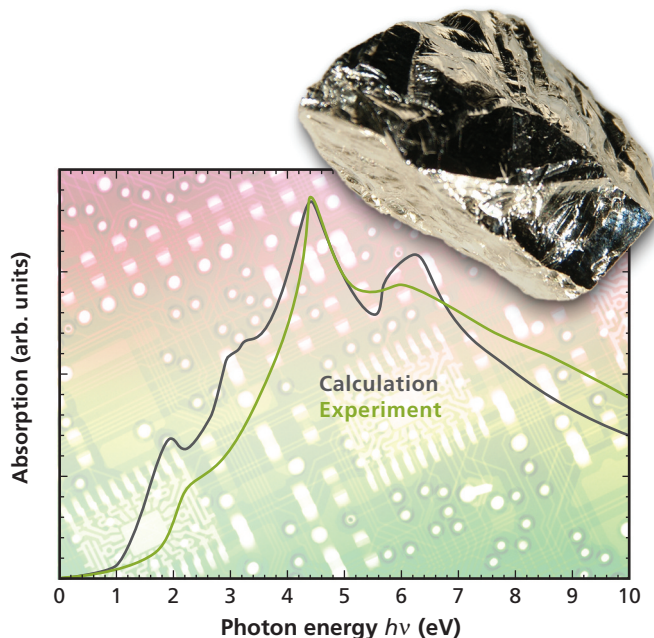
- Adsorption and Dissociation of Iodine Molecules on a Zr Surface
- Energy band structure of germanium
- Ferroelectric Properties of BaTiO_3

Visit our website www.materialsdesign.com or contact your local Materials Design office for further information.

Relevant Publications:

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

Germanium image credits: <http://images-of-elements.com/germanium.php>



Optical spectrum of Ge