materials design®

MedeA® VASP 5.4

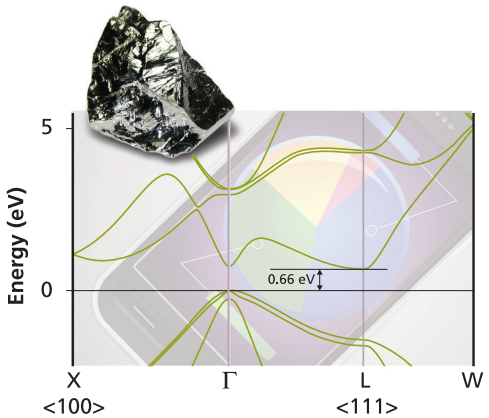
VASP 5.4 is the world leading first-principles solid state electronic structure program for solids, surfaces, and interfaces. Possessing a comprehensive array of advanced features, including hybrid functionals, the ability to incorporate dispersion interactions, and comprehensive and validated self-consistent PAW potentials, VASP 5.4 provides access to state-of-the-art first-principles simulation methods in a comprehensive and easy to use package. Advanced features include linear response calculations for properties such as Born effective charges, dielectric and piezoelectric tensors and NMR chemical shifts. VASP 5.4 is fully integrated in the MedeA® environment with graphical user interface driven model construction, efficient calculation execution, and analysis capabilities. VASP 5.4 enables the efficient computation of the following properties:

Properties from MedeA® VASP

- Total electronic energy of any 3D periodic arrangement of atoms
- Forces on atoms, pressure and stress tensors
- Collinear and non-collinear magnetic moments
- Equilibrium lattice parameters and atomic positions as obtained from energy, force and stress minimization
- Ab-initio molecular dynamics: nVE, nVT, npT ensembles, simulated annealing, trajectories
- 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 and spin density and electrostatic potential, Bader charge analysis
- Work functions
- Response functions including dielectric and piezoelectric tensors
- Born effective charges and Γ-point phonon modes
- Optical spectra: dielectric functions, refractive index and optical absorption as a function of frequency
- Hyperfine splitting
- Electric field gradients and quadrupolar coupling constants
- NMR chemical shifts

Computational Characteristics

- Plane-wave based electronic structure method for periodic structures
- All-electron method with projector augmented wave (PAW) potentials
- Scalar- and fully-relativistic, spin-orbit coupling
- Density functional theory (DFT) with local (LDA) and gradient-corrected (GGA) semi-local functionals: AM05, PBEsol, PBE, rPBE, BLYP, etc.
- Hybrid functionals: HSE06, PBE0, B3LYP, in addition screened exchange and Hartree-Fock
- Meta-GGA functionals: revTPSS, TPSS, M06-L, modified Becke-Johnson LDA
- Van-der-Waals functionals
- D2/D3-Grimme and Tkatchenko-Scheffler force-field based correction for van-der-Waals and dispersion forces and energies
- Solvation effects for surfaces and molecules



Tight Integration With

- *MedeA® Phonon 2.0*
- *MedeA® Electronics*
- *MedeA® Elastic Properties*
- *MedeA® Transition State Search*
- *MedeA® UNCLE (Cluster Expansion)*

Required MedeA® Modules

- *Core MedeA® Environment*
- *VASP Graphical User Interface*
- *JobServer & TaskServers*

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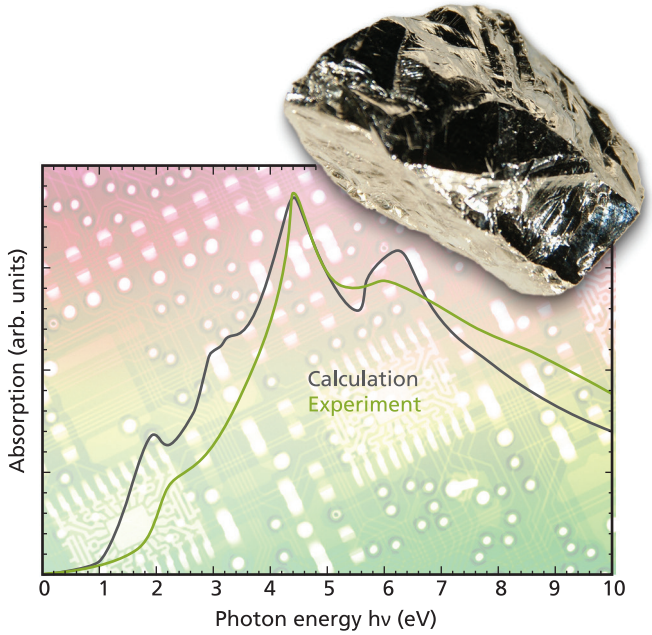
Full Integration

To accelerate calculations, intermediate results are used to improve the efficiency of subsequent steps. The MedeA® JobServer/TaskServer architecture provides efficient storage and deployment for temporary files and lets you focus on the science while computational book keeping and data storage is handled by the MedeA® infrastructure. MedeA® manages computational details, such as matching k-meshes and setting reasonable VASP parameters, automatically.



Tested, Validated, Optimized for High-Throughput

Materials Design® supports a wide array of hardware configurations with optimized and validated VASP executables. Windows and Linux versions allow you to mix and match of architectures, so you can run more calculations and with larger models on Linux clusters, confident that the results will be consistent with calculations executed on your laptop or desktop machines. The MedeA® environment enables both investigative and high throughput calculations, and the Materials Design® licensing model allows you to maximize parallel execution allowing you to exploit the growing availability of high performance compute resources and rapidly obtain state-of-the-art research results. As of MedeA® 2.21 VASP executables supporting GPUs are available.

More on our website:

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

Selected 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, vol. 78, p. 121201(R), 2008

*For further information, visit our website **www.materialsdesign.com** or contact us directly as given below.*

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