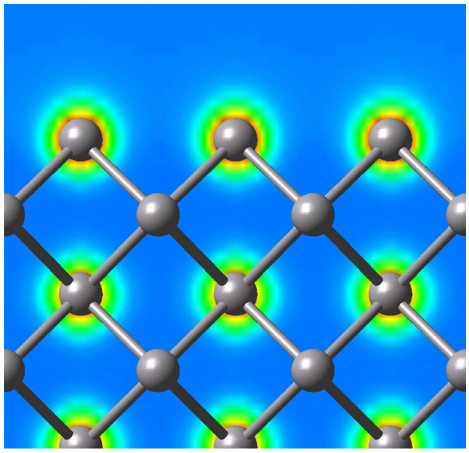
MedeA-VASP 4.6

The Vienna Ab initio Simulation Package (VASP) is a leading electronic structure program for solids, surfaces, and interfaces. Version 4.6 has become an extremely well tested, robust, and proven program for the calculation based on local and semi-local density functional theory. The program is fully integrated in the MedeA platform with a graphical user interface enabling the computation of the following properties:

Properties from VASP 4.6

- 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



Spin density on Fe(001) surface) computed with VASP 4.6 and rendered with MedeA's analysis tools.

- Energy band structure
- 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

Computational characteristics

- Plane-wave based electronic structure method for periodic structures
- All-electron frozen-core method with projector augmented wave (PAW) potentials
- Density functional theory (DFT) with local (LDA) and gradient-corrected (GGA) semi-local functionals
- Structure optimization by energy minimization using analytic first derivates (forces) and stress tensors
- Ab initio molecular dynamics

Other required MedeA modules

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

More on our website:

www.materialsdesign.com

- Modeling work function changes in CMOS stacks containing HfO_2 high-k dielectrics
- Structure of an iron oxide (Fe_2O_3) surface as function of temperature and O_2 pressure

Relevant Publications

- G Kresse and J Hafner, *Physical Review B Condensed Matter*, vol. 47, no. 1, p. 558, 1993.
- G Kresse and J Furthmüller, *Computational. Materials Science*, vol. 6, p. 15, 1996.
- G Kresse and J Furthmüller, *Physical Review B Condensed Matter*, vol. 54, no. 16, p. 11169, 1996