



WHAT IS NEW IN VASP5

Specialized Gradient Based Potentials

Solids: PBEsol AM05

These potentials are improvements of PBE and PW91 gradient-based potentials. Expect more accurate lattice parameters, elastic and vibrational properties.

Molecules and Surfaces: rPBE

Fine tuned for atomization energies of molecules and chemisorption on surfaces. This offers new perspectives in catalysis and molecular systems such as carbon nanotubes. Gather new insights in reaction kinetics with the new transition state module.

These new potentials are as fast as the PBE and PW potentials currently used in MEDEA and work with all modules.

Hybrid Functionals – Screened Exchange

PBE0 HSE06 B3LYP

Combining non-local exchange (Hartree-Fock) and density functional based exchange and correlation offers a successful alternative for systems with previously sizeable errors.

Experience a quantum leap to accurate band gaps, defect energies and optical properties. Screened exchange gives a better picture of magnetic materials and metal oxides based on a better description of the complex electronic structure.

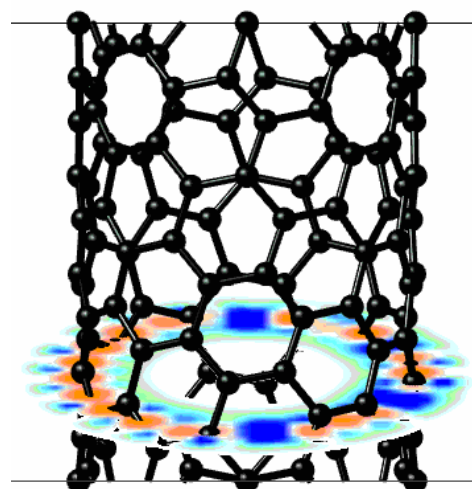
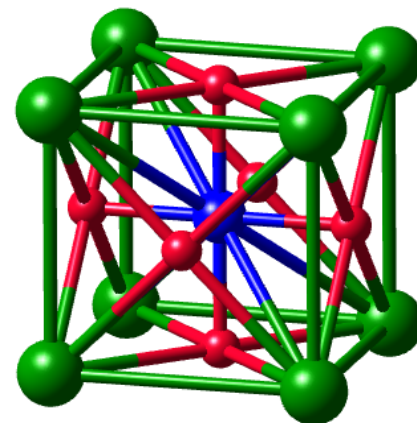
This comes with considerable computational demands as compared to gradient-based potentials.

TIME DEPENDENT DFT

VASP 5 opens the door to time dependent DFT.

Frequency Dependent Dielectric Functions

The frequency dependent dielectric functions (real and imaginary part) and the resulting optical spectra (absorption, reflection, transmission, refractive index) are available for insulators, semiconductors and metals.





Response Functions

VASP provides tensors based on analytical and numerical derivatives:

- Born effective charge tensor
- Dielectric constant tensor
- Interatomic force constants (dynamical matrix)
- Piezoelectric tensor

Frequency Dependent GW

One of the best approaches for accurate band gaps, dielectric functions and optical spectra. This quasiparticle method offers multiple stages of self-consistency.

Relaxed Core in PAW

Projecting back to the core and relaxing core electrons: This transforms VASP 5 into an all-electron full-potential code to access core levels, core level shifts and electric field gradients.

HOW DOES VASP 5 WORK IN MEDEA?

First Release

The most important features of VASP 5 are already fully supported in MEDEA, its graphical user interface, and its analysis tools. Expert features are accessible and your experience will shape the final interface.

Improved Gradient Based Potentials

Are supported by MEDEA like their siblings PBE and PW91. All combinations of +U methods, non-collinearity and spin-orbit coupling are available. VASP settings in Phonon and MT offer access to these new potentials.

Hybrid Functionals and Screened Exchange

Single point energy and structure optimization are fully supported.

Reference Energies

MEDEA provides rock solid reference data and safe default settings. Expect improvements while we populate the reference library.

Frequency Dependent Dielectric Function

Available right now. The complete optical analysis tool is coming up.