VASP versions in MedeA

Version VASP 5.4 is recommended for all VASP related applications, as accessed from the graphical user interfaces (GUI) of VASP 5.4, Phonon, *MT*, *Electronics*, *TSS*, *Automated Convergence*, *Point Defect Analysis* and within Flowcharts.

The VASP 5.4 GUI applies VASP 5.4.4 executables and the new and improved set of PAW potentials (published September 4, 2015) including the second generation of specialized potentials for more accurate treatment of excited states (GW potentials), created with the LDA and GGA-PBE exchange correlation functionals.

Functionals

Given that no functional is best for all possible applications, a whole range of advanced descriptions for the inter-atomic interactions is available:

- In addition to the widely applied standard approximations to exchange and correlation, LDA and GGA-PBE, a number of additional GGA functionals is provided.
- Furthermore, a variety of meta-GGA functionals for more accurate total energies or band energies is available.
- Van der Waals potentials for an approximate ab-initio treatment of dispersive forces can be applied, or alternatively a forcefield based coverage of van der Waals interactions can be pursued.
- For an improved description of excited states including its consequences for the energy, the non-local exchange based functionals (hybrid functionals, screened exchange and Hartree-Fock) can be selected, or extremely demanding GW calculations can be performed. Electron-hole interaction for excitonic effects are captured by solving the Bethe-Salpeter equation or from time-dependent DFT.
- Accurate total energies can be evaluated by adding exact exchange energies and accurate correlation energies from the adiabatic connection fluctuation dissipation theorem (ACFDT) within the random phase approximation (RPA).

In terms of magnetic interactions, a collinear (spin-polarized), non-collinear or fully relativistic (spin-orbit split) description is available.

Capabilities

VASP 5.4 allows single point energy, geometry optimization and molecular dynamics simulations, and calculation of a number of properties such as electronic densities of states, band structures, charge densities, charge decompositions, electron localization functions and the local potential, optical spectra, response tensors (dielectric and piezoelectric tensors and Born effective charges), zone center phonon modes, electric field gradients at the nuclei positions, hyperfine parameters characterizing the interactions between the spin of nuclei with the electronic spin densities, chemical shifts as derived in nuclear magnetic resonance (NMR) spectroscopy, and work functions for surfaces. For molecules and surfaces solvent effects can be captured by means of an implicit solvation model. Further properties are available from other modules making use of VASP 5.4.

Why should I not switch to VASP 5.4?

VASP 5.4 makes use of the new potentials and is strongly recommended. Due to the differences in energies, for projects started with older VASP versions we suggest two possible routes:

- For extensive projects underway, continue to use an older version of *MedeA* with VASP 5.2 (or VASP 4.6) and old potentials.
- For anything else, reuse “old” structures with VASP 5.4 applying the new, improved potentials, which may involve recalculating the energy for previous structures, and for optimization checking forces and stresses to see whether they are acceptable or require continued optimization.