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VASP versions in MedeA

Version VASP 6 is recommended for all VASP related applications, as accessed from the graphical user interfaces (GUI) of VASP 6, Phonon, *MT*, *Electronics*, *TSS*, *Automated Convergence*, *Point Defect Analysis* and within Flowcharts.

The VASP 6 GUI applies VASP 6.3.2 executables and the most recent and optimized 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, Advanced Simulation Techniques

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

- In addition to the widely applied standard approximations to exchange and correlation, LDA and GGA-PBE, several additional GGA functionals are provided.

- Furthermore, a variety of meta-GGA functionals for more accurate total energies or band energies is available.

- Van der Waals functionals for an approximate ab-initio treatment of dispersive forces can be applied, or 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.

- Highest level of accuracy for excited states and optical properties can be obtained from extremely demanding GW quasiparticle calculations. Electron-hole interactions for excitonic effects are captured by solving the Bethe-Salpeter equation on top of a GW calculation or from time-dependent DFT, optionally combined with a model Bethe-Salpeter approach. An alternative route to accurate optical spectra is provided by means of the Time Evolution methodology.

- 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).

- Both for GW and ACFDT calculations the space-time approach for calculating the polarizability can be applied, which scales essentially cubic in system size (rather than quartic), as such allowing the study of relatively large systems.

- Accurate total energies, forces, and phonon modes from adiabatic connection applying the space-time algorithm (Low Scaling ACFDT-RPA). There is a T=0 K approach suitable for semiconductors and insulators, as well as a final temperature approach applicable also for metals. Based on the accurate forces optimization of atom positions becomes feasible.

- The final temperature approach for metals is also available for low scaling GW simulations.

- Electron-phonon coupling at a given temperature using stochastic displacements of atoms is a further available feature of VASP 6. Both a one-shot displacement configuration (following the approach of M. Zacharias and F. Giustino) and a full Monte Carlo sampling of configurations for a given temperature are available.

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- Create a forcefield by on-the-fly machine-learning during ab-initio molecular dynamics simulations, which can thereby be extended to much larger time lengths due to replacing ab-initio steps by forcefiled-based steps. Making use of such machine-learned forcefields, various simulation types can be extended to much larger system sizes, as well.

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

Capabilities

VASP 6 allows single point energy, geometry optimization and molecular dynamics simulations, and calculation of several 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 and external electric field can be applied. In addition, *MedeA VASP 6* offers automatic procedures to evaluate energies of formation, referenced to the elements in their standard state. Further properties are available from other modules making use of VASP 6.

Why should I not switch to MedeA VASP 6?

VASP 6 makes use of the latest set of potentials and is strongly recommended. Since total energies are unchanged between VASP 5.4 and VASP 6, and both program versions use the same set of most recent potentials, there are no worries concerning compatibility between these two VASP versions. However, for projects started with even older VASP versions than VASP 5.4 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 6 applying the more recent, 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.

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