Standards and Reference Energies

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1 The *MedeA* Standard 500

MedeA has introduced a standard for the Precision of VASP calculations, automatically applying *PREC = Accurate* and a plane wave cutoff of 500 eV (900 eV for hard potentials with *ENMAX* $>$ 450 eV). *Standard 500* is recommended in cases where an overall precise plane cutoff and setting is required for a single system or for a range of systems with varying constituent elements. Using a standard cutoff of 500eV within a project has the advantage of facilitating the comparison of data from compounds containing different elements like e.g. in the calculation of heat of formations or defect energies.

VASP parameters covered by Precision *Standard 500*:

- Precision accurate
- Planewave cutoff 500eV (900 eV for hard potentials with *ENMAX* $>$ 450 eV)

VASP parameters recommended to be set in addition, to comply with *Standard 500*:

- Reciprocal space projection
- Convergence criterion for SCF cycle: 10^{-7} eV
- Convergence criterion for geometry optimization: 0.001 eV/Å
- Conjugate gradient geometry optimization

For crystalline structures:

- k-spacing of 0.2 Å^{-1}, Shift origin to Gamma
- For non-local exchange based functionals (e.g. hybrid functionals): k-spacing of 0.5 Å^{-1}, Shift origin to Gamma, X, Y, and Z axis k-mesh factors all set to 2
- Tetrahedron method including Blöchl corrections

For molecular structures:

- Box ensuring a minimum of about 8 Å empty space between the molecule and its symmetry copies in all directions
- Γ-point only
- Fermi smearing with 0 eV smearing width

2 Reference Energies for the Calculation of the Heat of Formation

The computation of the electronic contribution to heats of formation for compounds requires reference energies for all constituent elements in their standard state. Below is a list of model structures for all ele-

ments in their standard state, which is applied for calculating the Energy of formation as a property from the *MedeA VASP 6 GUI*. For a few cases the standard state structure is replaced by a different structure together with a correction energy. For the structure optimization calculations for the reference systems, in general a non-magnetic Hamiltonian is used, however, spin-polarization is required for O_2, Cr(antiferromagnetic), γ-Mn(antiferromagnetic), Fe, Co, Ni, and lanthanides heavier than Ce for potentials including *f* electrons as valence states. For solids, all cell parameters and internal degrees of freedom need to be relaxed. For atoms and molecules a fixed box of 10 $\mathring{A}$ in each dimension is used (for S_8 molecules a cubic box of 15 $\mathring{A}$), for molecules the atomic positions need to be relaxed. For computing energies of formation, the application of *Standard 500* settings as outlined above are recommended to obtain suitable accuracy.

Table1: Summary of models and technical details for the calculations of reference energies of the elements

Elements	Structure	Correction, techn. details
H	H_2 molecule	
He	He atom	
Li	bcc	
Be	α-Be, hcp	
B	α-B, R-3m	
C	diamond, Fd-3m	-1.897 kJ/mol, because graphite is low temperature phase
N	N_2 molecule	
O	O_2 molecule	spin-polarized, because molecule exists in triplet state
F	F_2 molecule	
N	Ne atom	
Na	bcc	
Mg	hcp	
Al	fcc	
Si	Fd-3m	
P	Cmca, black phosphorus	
S	S_8 molecule	-13.04875 kJ/mol, condensation
Cl	Cl_2 molecule	
Ar	Ar atom	
K	bcc	
Ca	α-Ca, fcc	
Sc	α-Sc, hcp	
Ti	α-Ti, hcp	
V	bcc	
Cr	α-Cr, bcc, antiferromagnetic	spin-polarized
Mn	γ-Mn P4/mmm, antiferromagnetic	-4.348 kJ/mol = α-Mn, spin-polarized
Fe	α-Fe, bcc	spin-polarized
Co	β-Co, hcp	spin-polarized
Ni	fcc	spin-polarized
Cu	fcc	
Zn	hcp	
Ga	α-Ga, Cmca	
Ge	Fd-3m	
As	R-3m	grey metallic
Se	P3121	grey metallic
Br	Br_2 molecule	-22.85 kJ/mol, condensation
Kr	Kr atom	
Rb	bcc	
Sr	α-Sr, fcc	
Y	hcp	
Zr	α-Zr, hcp	
Nb	bcc	

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Elements	Structure	Correction, techn. details
Mo	bcc	
Tc	hcp	
Ru	hcp	
Rh	fcc	
Pd	fcc	
Ag	fcc	
Cd	hcp	
In	I4/mmm	
Sn	α-Sn, Fd-3m	transition temperature of 286 K to β-Sn, I41/amd
Sb	R-3m	
Te	P3121	
I	Cmca	
Xe	Xe atom	
Cs	bcc	
Ba	bcc	
La	α-La, dhcp	
Ce	γ-Ce, fcc	
Pr	dhcp	
Nd	dhcp	
Pm	dhcp	
Sm	R-3m	
Eu	bcc	
Gd	hcp	
Tb	hcp	
Dy	hcp	
Ho	hcp	
Er	hcp	
Tm	hcp	
Yb	fcc	
Lu	hcp	
Hf	hcp	
Ta	α-Ta, bcc	
W	α-W, bcc	
Re	hcp	
Os	hcp	
Ir	fcc	
Pt	fcc	
Au	fcc	
Hg	R-3m	2.3 kJ/mol melting (JANAF)
Tl	α-Tl, hcp	
Pb	fcc	
Bi	R-3m	
Po	Pm-3m	
At	no structure	
Rn	Rn atom	
Fr	no structure	
Ra	bcc	
Ac	fcc	
Th	α-Th, fcc	
Pa	I4/mmm	
U	α-U, Cmcm	
Np	Pnma	
Pu	α-Pu, P121/m1	

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Table 1 – continued from previous page

Elements	Structure	Correction, techn. details
Am	dhcp	
Cm	dhcp	