Standards and Reference Energies

Contents

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/$\mathrm{\AA}$
- Conjugate gradient geometry optimization

For crystalline structures:

- k-spacing of 0.2 $\mathrm{\AA}$ -1, odd size grids
- Tetrahedron method including Bl$\ddot{o}$ chl corrections

For molecular structures:

- Box ensuring a minimum of about 8 $\mathrm{\AA}$ 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 recommended model structures for all elements in their standard state, or a replacement together with a correction energy. The above complete *Standard 500* settings are recommended, with non-magnetic Hamiltonian in general, however, spin-polarized

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 Åin each dimension is used (for S8 molecules a cubic box of 15 Å), for molecules the atomic positions need to be relaxed.

Element	**Structure**	**Correction, technical details**
H	H_2molecule	
He	He atom	
Li	bcc	
Be	α-Be, hcp	
B	α-B, R-3m	
C	Diamond, Fd-3m	-1.897 kJ/mol = graphite
N	N_2molecule	
O	O_2molecule, FM	
F	F_2molecule	
Ne	Ne atom	
Na	bcc	
Mg	hcp	
Al	fcc	
Si	Fd-3m	
P	Black phosphorus	
S	S8 molecule	-13.04875 kJ/mol condensation
Cl	Cl_2molecule	
Ar	Ar atom	
K	bcc	
Ca	α-Ca, fcc	
Sc	α-Sc, hcp	
Ti	α-Ti, hcp	
V	bcc	
Cr	α-Cr, bcc,	
Mn	γ-Mn P4/mmm	-4.348 kJ/mol
Fe	α-Fe, bcc,	
Co	β-Co, hcp,	
Ni	fcc, FM	
Cu	fcc	
Zn	hcp	
Ga	α-Ga, Cmca	
Ge	Fd-3m	
As	R-3m	grey metallic
Se	P3121	grey metallic
Br	Br2 molecule	-22.85 kJ/mol condensation

DOCUMENTATION

Kr. . . . . Kr atom. . . . . .
Rb. . . . . bcc . . . . . .
Sr. . . . . α-Sr, fcc. . . . . .
Y. . . . . hcp . . . . . .
Zr. . . . . α-Zr, hcp. . . . . .
Nb. . . . . bcc . . . . . .
Mo. . . . . bcc . . . . . .
Tc. . . . . hcp . . . . . .
Ru. . . . . hcp . . . . . .
Rh. . . . . fcc . . . . . .
Pd. . . . . fcc . . . . . .
Ag. . . . . Silver 3C. . . . . .
Cd. . . . . hcp . . . . . .
In. . . . . I4/mmm . . . .
Sn. . . . . α-Sn, Fd-3m. . . . . transition temperature 286K
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. . . . . no potential. . . . . ..
At. . . . . no potential. . . . . ..
Rn. . . . . no potential. . . . . ..
Fr. . . . . no potential. . . . . ..
Ra. . . . . no potential. . . . . ..
Ac. . . . . fcc . . . . . .
Th. . . . . α-Th, fcc. . . . . .
Pa. . . . . I4/mmm . . . .
U. . . . . .. α-U, Cmcm. . . . . .
Np. . . . . no potential. . . . . ..
Pu. . . . . in progress. . . . . .