

==> INCAR <==

NELMDL = -4
SIGMA = 0.1
EDIFF = 1e-5
GGA = PE
NPAR = 8
ISMEAR = 0
ENCUT = 450
LWAVE = .FALSE.
LCHARG = .FALSE.
ISPIN = 1
NELM = 200
AMIX = 0.2

==> KPOINTS <==

Automatic mesh

0
A
25

==> KPOINTS_gamma <==

Automatic mesh

0
G
1 1 1
0 0 0

==> POTCAR.Au <==

PAW_PBE Au 06Sep2000
11.0000000000000000
parameters from PSCTR are:
VRHFIN = Au: s1d10
LEXCH = PE
EATOM = 926.0567 eV, 68.0632 Ry

TITEL = PAW_PBE Au 06Sep2000
LULTRA = F use ultrasoft PP ?
IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no
RPACOR = 2.330 partial core radius
POMASS = 196.966; ZVAL = 11.000 mass and valenz
RCORE = 2.500 outmost cutoff radius
RWIGS = 2.840; RWIGS = 1.503 wigner-seitz radius (au A)
ENMAX = 229.948; ENMIN = 172.461 eV
RCLOC = 1.964 cutoff for local pot
LCOR = T correct aug charges
LPAW = T paw PP
EAUG = 356.670
DEXC = -.025
RMAX = 3.041 core radius for proj-oper
RAUG = 1.300 factor for augmentation sphere
RDEP = 2.598 radius for radial grids
QCUT = -4.111; QGAM = 8.222 optimization parameters

Description

	1	E	TYP	RCUT	TYP	RCUT
	2	.000	23	2.500		
	2	.000	23	2.500		

```

0 .000 23 2.500
0 .000 23 2.500
1 -.200 23 2.500
1 .000 23 2.500
3 .000 7 .000
Error from kinetic energy argument (eV)
NDATA = 100
STEP = 20.000 1.050
212. 208. 207. 203. 201. 197. 192. 190.
185. 180. 178. 173. 167. 161. 156. 150.
144. 137. 131. 122. 116. 110. 101. 94.9
89.1 80.6 72.6 67.4 60.0 53.1 46.6 40.7
35.2 30.3 25.8 21.8 17.2 14.3 10.9 8.81
6.52 4.71 3.32 2.28 1.52 .979 .610 .325
.194 .107 .716E-01 .621E-01 .598E-01 .594E-01 .559E-01 .495E-01
.409E-01 .299E-01 .202E-01 .131E-01 .870E-02 .659E-02 .590E-02 .580E-02

```

==> POTCAR.O <==

PAW_PBE O 08Apr2002

6.000000000000000000

parameters from PSCTR are:

VRHFIN =O: s2p4

LEXCH = PE

EATOM = 432.3788 eV, 31.7789 Ry

TITEL = PAW_PBE O 08Apr2002

LULTRA = F use ultrasoft PP ?

IUNSCR = 0 unscreen: 0-lin 1-nonlin 2-no

RPACOR = .000 partial core radius

POMASS = 16.000; ZVAL = 6.000 mass and valenz

RCORE = 1.520 outmost cutoff radius

RWIGS = 1.550; RWIGS = .820 wigner-seitz radius (au A)

ENMAX = 400.000; ENMIN = 300.000 eV

ICORE = 2 local potential

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 605.392

DEXC = .000

RMAX = 2.264 core radius for proj-oper

RAUG = 1.300 factor for augmentation sphere

RDEP = 1.550 radius for radial grids

QCUT = -5.520; QGAM = 11.041 optimization parameters

Description

1 E TYP RCUT TYP RCUT

0 .000 23 1.200

0 -.700 23 1.200

1 .000 23 1.520

1 .600 23 1.520

2 .000 7 1.500

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

163. 160. 159. 156. 154. 151. 148. 146.

142. 139. 137. 134. 130. 126. 123. 119.

115. 111. 108. 102. 98.8 95.2 90.0 86.6

83.2	78.3	73.5	70.4	65.9	61.6	57.4	53.4
49.6	46.0	42.6	39.3	35.3	32.4	28.9	26.4
23.4	20.6	18.1	15.8	13.7	11.9	10.3	8.47
7.22	5.87	4.73	3.95	3.13	2.45	1.80	1.37
1.03	.721	.493	.329	.215	.138	.882E-01	.534E-01
.367E-01	.267E-01	.223E-01	.205E-01	.193E-01	.181E-01	.162E-01	.138E-01

```

==> POTCAR.Ti <==
PAW_PBE Ti 08Apr2002
4.000000000000000
parameters from PSCTR are:
VRHFIN =Ti: d3 s1
LEXCH = PE
EATOM = 94.7928 eV, 6.9671 Ry

TITEL = PAW_PBE Ti 08Apr2002
LULTRA = F use ultrasoft PP ?
IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no
RPACOR = 2.200 partial core radius
POMASS = 47.880; ZVAL = 4.000 mass and valenz
RCORE = 2.800 outmost cutoff radius
RWIGS = 2.500; RWIGS = 1.323 wigner-seitz radius (au A)
ENMAX = 178.330; ENMIN = 133.747 eV
RCLOC = 2.215 cutoff for local pot
LCOR = T correct aug charges
LPAW = T paw PP
EAUG = 328.883
DEXC = 0.000
RMAX = 2.868 core radius for proj-oper
RAUG = 1.300 factor for augmentation sphere
RDEP = 2.885 radius for radial grids
RDEPT = 2.320 core radius for aug-charge

```

Atomic configuration

```

9 entries
n l j      E      occ.
1 0 0.50 -4865.3608 2.0000
2 0 0.50 -533.1367 2.0000
2 1 1.50 -440.5031 6.0000
3 0 0.50 -59.3186 2.0000
3 1 1.50 -35.7012 6.0000
3 2 2.50 -1.9157 3.0000
4 0 0.50 -3.7291 1.0000
4 1 1.50 -4.0817 0.0000
4 3 2.50 -1.3606 0.0000

```

```

Description
1 E      TYP RCUT  TYP RCUT
2 -1.9156924 23 2.800
2 -0.4062961 23 2.800
0 -3.7290832 23 2.800
0 20.4087390 23 2.800
1 -5.4423304 23 2.800

```

```

Error from kinetic energy argument (eV)
NDATA = 100
STEP = 20.000 1.050
27.5 26.6 26.1 25.2 24.7 23.7 22.7 22.2

```

21.2	20.2	19.7	18.7	17.7	16.7	15.7	14.7
13.8	12.9	12.0	10.7	9.91	9.13	8.02	7.33
6.68	5.77	4.94	4.43	3.74	3.12	2.58	2.11
1.71	1.36	1.07	0.834	0.581	0.434	0.286	0.204
0.126	0.745E-01	0.425E-01	0.240E-01	0.143E-01	0.984E-02	0.823E-02	0.787E-02
0.783E-02	0.744E-02	0.653E-02	0.554E-02	0.420E-02	0.297E-02	0.185E-02	0.126E-02

```

==> POTCAR.C <==
PAW_PBE C 08Apr2002
4.000000000000000
parameters from PSCTR are:
VRHFIN =C: s2p2
LEXCH = PE
EATOM = 147.1560 eV, 10.8157 Ry

TITEL = PAW_PBE C 08Apr2002
LULTRA = F use ultrasoft PP ?
IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no
RPACOR = 1.200 partial core radius
POMASS = 12.011; ZVAL = 4.000 mass and valenz
RCORE = 1.500 outmost cutoff radius
RWIGS = 1.630; RWIGS = 0.863 wigner-seitz radius (au A)
ENMAX = 400.000; ENMIN = 300.000 eV
ICORE = 2 local potential
LCOR = T correct aug charges
LPAW = T paw PP
EAUG = 644.873
DEXC = 0.000
RMAX = 1.529 core radius for proj-oper
RAUG = 1.300 factor for augmentation sphere
RDEP = 1.501 radius for radial grids
RDEPT = 1.300 core radius for aug-charge

```

Atomic configuration

4 entries

n	l	j	E	occ.
1	0	0.50	-273.3789	2.0000
2	0	0.50	-13.7508	2.0000
2	1	0.50	-5.2854	2.0000
3	2	1.50	-5.4423	0.0000

Description

l	E	TYP	RCUT	TYP	RCUT
0	-13.7508458	23	1.200		
0	-8.2022199	23	1.200		
1	-5.2854383	23	1.500		
1	34.0145650	23	1.500		
2	-5.4423304	7	1.500		

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

51.3	49.5	48.6	46.8	45.9	44.1	42.4	41.6
39.9	38.2	37.4	35.8	34.3	32.8	31.4	30.0
28.6	27.3	26.1	24.3	23.2	22.1	20.5	19.6
18.6	17.3	16.0	15.2	14.1	13.1	12.1	11.1
10.3	9.47	8.72	8.02	7.15	6.55	5.82	5.31
4.69	4.13	3.63	3.17	2.76	2.40	2.07	1.72

1.47 1.20 0.971 0.815 0.650 0.512 0.380 0.292
0.222 0.158 0.110 0.748E-01 0.504E-01 0.337E-01 0.227E-01 0.149E-01
0.111E-01 0.869E-02 0.756E-02 0.700E-02 0.657E-02 0.614E-02 0.551E-02 0.474E-02

==> POTCAR.H <==

PAW_PBE H 15Jun2001

1.000000000000000000

parameters from PSCTR are:

VRHFIN =H: ultrasoft test

LEXCH = PE

EATOM = 12.4884 eV, .9179 Ry

TITEL = PAW_PBE H 15Jun2001

LULTRA = F use ultrasoft PP ?

IUNSCR = 0 unscreen: 0-lin 1-nonlin 2-no

RPACOR = .000 partial core radius

POMASS = 1.000; ZVAL = 1.000 mass and valenz

RCORE = 1.100 outmost cutoff radius

RWIGS = .700; RWIGS = .370 wigner-seitz radius (au A)

ENMAX = 250.000; ENMIN = 200.000 eV

RCLOC = .701 cutoff for local pot

LCOR = T correct aug charges

LPAW = T paw PP

EAUG = 400.000

RMAX = 2.174 core radius for proj-oper

RAUG = 1.200 factor for augmentation sphere

RDEP = 1.112 radius for radial grids

QCUT = -5.749; QGAM = 11.498 optimization parameters

Description

1 E TYP RCUT TYP RCUT

0 .000 23 1.100

0 .500 23 1.100

1 -.300 23 1.100

Error from kinetic energy argument (eV)

NDATA = 100

STEP = 20.000 1.050

5.77 5.50 5.37 5.11 4.99 4.75 4.52 4.40

4.19 3.98 3.88 3.68 3.49 3.31 3.14 2.98

2.83 2.68 2.54 2.35 2.22 2.11 1.94 1.84

1.74 1.61 1.48 1.40 1.29 1.19 1.09 1.01

.925 .851 .782 .719 .642 .590 .526 .482

.430 .382 .339 .301 .267 .236 .209 .178

.157 .133 .113 .988E-01 .832E-01 .697E-01 .562E-01 .467E-01

.386E-01 .305E-01 .239E-01 .186E-01 .143E-01 .109E-01 .820E-02 .580E-02