VASP2007/VASP

VASP 2007 PAW dataset / VASP 5.2.2

`name and version of the code:` VASP 5.2.2
`type of basis set:` plane waves
`method:` projector-augmented wave (VASP 2007)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core fully relativistic valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table I (valence Z_{val})
`basis set size`	see table I (cutoff energy E_{cut})
`k-mesh density`	see table I (k-point grid *kpts* in the full 1st Brillouin zone of the primitive (*) or conventional cell)
`reciprocal-space integration method`	Blöchl tetrahedron method

METHOD-SPECIFIC INFORMATION

`FFT grid`	wavevectors up to $2\,G_{cut} = 2\sqrt{\frac{2m_e E_{cut}}{\hbar^2}}$ included
`augmentation charge grid`	wavevectors up to $4\,G_{cut}$ included

ADDITIONAL COMMENTS

none

REFERENCES

`PAW dataset`

[1] G. Kresse, D. Joubert, *Phys. Rev. B* **59**, 1758–1775 (1999).

`code`

[2] G. Kresse, J. Furthmüller, *Comput. Mater. Sci.* **6**, 15–50 (1996).
[3] J. Hafner, *J. Comput. Chem.* **29**, 2044–2078 (2008).

`scalar relativity`

[4] D. D. Koelling and B. N. Harmon, *J. Phys. C: Solid State* **10**, 3107–3114 (1977).

`reciprocal-space integration`

[5] P. E. Blöchl, O. Jepsen and O. K. Andersen, *Phys. Rev. B* **49**, 16223–16234 (1977).

Table I. Calculation settings per element: PAW potential, valence Z_{val}, cutoff energy E_{cut}, k-mesh in the full 1st Brillouin zone of the conventional cell *kpts* (of the primitive cell for elements with an asterisk*).

	potential	Z_{val} [–]	E_{cut} [eV]	*kpts* [–]
H	PAW_PBE H 15Jun2001	1	400	15 × 15 × 11
He	PAW_PBE He 05Jan2001	2	600	21 × 21 × 11
Li*	PAW_PBE Li_sv 23Jan2001	3	400	15 × 15 × 15
Be	PAW_PBE Be 06Sep2000	2	400	21 × 21 × 11
B*	PAW_PBE B 06Sep2000	3	600	9 × 9 × 9
C	PAW_PBE C 08Apr2002	4	600	17 × 17 × 9
N	PAW_PBE N 08Apr2002	5	600	11 × 11 × 11
O	PAW_PBE O 08Apr2002	6	600	15 × 15 × 13
F	PAW_PBE F 08Apr2002	7	600	9 × 13 × 7
Ne	PAW_PBE Ne 05Jan2001	8	600	13 × 13 × 13
Na*	PAW_PBE Na_pv 05Jan2001	7	400	15 × 15 × 15
Mg	PAW_PBE Mg 05Jan2001	2	400	21 × 21 × 11
Al	PAW_PBE Al 04Jan2001	3	400	13 × 13 × 13
Si*	PAW_PBE Si 05Jan2001	4	400	15 × 15 × 15
P	PAW_PBE P 17Jan2003	5	400	15 × 5 × 11
S	PAW_PBE S 17Jan2003	6	400	19 × 19 × 19
Cl	PAW_PBE Cl 17Jan2003	7	400	13 × 13 × 13
Ar	PAW_PBE Ar 07Sep2000	8	400	13 × 13 × 13
K	PAW_PBE K_sv 06Sep2000	9	400	15 × 15 × 15
Ca	PAW_PBE Ca_pv 06Sep2000	8	400	13 × 13 × 13
Sc	PAW_PBE Sc_sv 07Sep2000	11	400	21 × 21 × 11
Ti	PAW_PBE Ti_pv 07Sep2000	10	400	21 × 21 × 11
V	PAW_PBE V_pv 07Sep2000	11	400	15 × 15 × 15
Cr	PAW_PBE Cr_pv 07Sep2000	12	400	15 × 15 × 15
Mn	PAW_PBE Mn_pv 07Sep2000	13	400	13 × 13 × 13
Fe	PAW_PBE Fe 06Sep2000	8	400	15 × 15 × 15
Co	PAW_PBE Co 06Sep2000	9	400	15 × 15 × 15
Ni	PAW_PBE Ni 06Sep2000	10	400	13 × 13 × 13
Cu	PAW_PBE Cu 05Jan2001	11	400	13 × 13 × 13
Zn	PAW_PBE Zn 06Sep2000	12	400	21 × 21 × 11
Ga	PAW_PBE Ga_d 06Sep2000	13	400	11 × 11 × 11
Ge*	PAW_PBE Ge_d 06Sep2000	14	400	15 × 15 × 15
As	PAW_PBE As 06Sep2000	5	400	17 × 17 × 7
Se	PAW_PBE Se 06Sep2000	6	400	13 × 13 × 13
Br	PAW_PBE Br 06Sep2000	7	400	13 × 13 × 13
Kr	PAW_PBE Kr 07Sep2000	8	400	13 × 13 × 13
Rb	PAW_PBE Rb_sv 06Sep2000	9	400	15 × 15 × 15
Sr	PAW_PBE Sr_sv 07Sep2000	10	400	13 × 13 × 13
Y	PAW_PBE Y_sv 06Sep2000	11	400	21 × 21 × 11
Zr	PAW_PBE Zr_sv 07Sep2000	12	400	21 × 21 × 11
Nb	PAW_PBE Nb_pv 08Apr2002	11	400	15 × 15 × 15
Mo	PAW_PBE Mo_pv 08Apr2002	12	400	15 × 15 × 15
Tc	PAW_PBE Tc_pv 06Sep2000	13	400	21 × 21 × 11
Ru	PAW_PBE Ru 06Sep2000	8	400	21 × 21 × 11
Rh	PAW_PBE Rh 06Sep2000	9	400	13 × 13 × 13
Pd	PAW_PBE Pd 05Jan2001	10	400	13 × 13 × 13
Ag	PAW_PBE Ag 06Sep2000	11	400	13 × 13 × 13
Cd	PAW_PBE Cd 06Sep2000	12	400	21 × 21 × 11

In	PAW_PBE In_d 06Sep2000	13	400	19 × 19 × 13
Sn*	PAW_PBE Sn_d 06Sep2000	14	400	15 × 15 × 15
Sb	PAW_PBE Sb 06Sep2000	5	400	17 × 17 × 7
Te	PAW_PBE Te 08Apr2002	6	400	13 × 13 × 13
I	PAW_PBE I 08Apr2002	7	400	13 × 13 × 13
Xe	PAW_PBE Xe 07Sep2000	8	400	13 × 13 × 13
Cs	PAW_PBE Cs_sv 08Apr2002	9	400	15 × 15 × 15
Ba	PAW_PBE Ba_sv 06Sep2000	10	400	15 × 15 × 15
Lu	PAW_PBE Lu_3 06Sep2000	9	400	21 × 21 × 11
Hf	PAW_PBE Hf_pv 06Sep2000	10	400	21 × 21 × 11
Ta	PAW_PBE Ta_pv 07Sep2000	11	400	15 × 15 × 15
W	PAW_PBE W_pv 06Sep2000	12	400	15 × 15 × 15
Re	PAW_PBE Re 17Jan2003	7	400	21 × 21 × 11
Os	PAW_PBE Os_pv 20Jan2003	14	400	21 × 21 × 11
Ir	PAW_PBE Ir 06Sep2000	9	400	13 × 13 × 13
Pt	PAW_PBE Pt 05Jan2001	10	400	13 × 13 × 13
Au	PAW_PBE Au 06Sep2000	11	400	13 × 13 × 13
Hg	PAW_PBE Hg 06Sep2000	12	400	15 × 15 × 15
Tl	PAW_PBE Tl_d 06Sep2000	13	400	21 × 21 × 11
Pb	PAW_PBE Pb_d 06Sep2000	14	400	13 × 13 × 13
Bi	PAW_PBE Bi_d 06Sep2000	15	400	17 × 17 × 7
Po	PAW_PBE Po_d 25May2007	16	400	19 × 19 × 19
Rn	PAW_PBE Rn 28Aug2006	8	400	13 × 13 × 13

Table II. Calculation results per element: equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	17.445	10.101	3.032
He	17.721	0.923	7.416
Li	20.286	13.801	3.159
Be	7.920	123.305	3.293
B	7.251	237.006	3.467
C	11.661	208.405	3.558
N	29.648	56.413	3.859
O	19.186	51.428	4.058
F	19.541	34.185	4.203
Ne	24.606	1.071	14.475
Na	37.074	7.688	3.044
Mg	22.847	36.471	3.919
Al	16.487	77.287	4.651
Si	20.446	88.790	4.296
P	21.359	68.513	4.338
S	17.167	83.524	4.136
Cl	38.207	19.154	4.334
Ar	52.652	0.788	7.351
K	73.844	3.592	3.818
Ca	42.169	17.518	3.017
Sc	24.659	54.370	3.406
Ti	17.371	112.521	3.599
V	13.484	181.621	4.020
Cr	11.834	176.751	7.166
Mn	11.569	115.449	0.354
Fe	11.375	185.742	4.910
Co	10.875	210.783	4.994
Ni	10.942	193.681	4.919
Cu	12.026	136.757	5.097
Zn	15.288	74.193	5.624
Ga	20.356	48.928	5.087
Ge	23.911	58.826	4.777
As	22.686	68.726	4.294
Se	29.829	47.229	4.480
Br	39.467	22.463	4.850
Kr	66.559	0.683	4.824
Rb	91.238	2.790	3.729
Sr	54.541	11.132	4.594
Y	32.921	41.378	3.203
Zr	23.530	93.781	3.584
Nb	18.337	171.753	3.970
Mo	15.917	262.885	4.342
Tc	14.596	298.498	4.545
Ru	13.844	311.518	4.951
Rh	14.179	254.234	5.250
Pd	15.444	168.191	5.636
Ag	18.054	89.106	5.778
Cd	23.008	43.780	7.225
In	27.538	35.433	5.335

Sn	36.859	35.843	4.852
Sb	31.794	50.899	4.544
Te	34.961	44.964	4.721
I	50.123	18.720	5.090
Xe	87.770	0.525	7.764
Cs	116.957	1.974	3.483
Ba	63.554	8.863	3.107
Lu	29.469	47.159	3.438
Hf	22.496	107.831	3.478
Ta	18.325	194.286	3.972
W	16.226	304.396	4.298
Re	14.933	372.481	4.548
Os	14.360	400.928	4.948
Ir	14.566	345.973	5.173
Pt	15.723	248.060	5.534
Au	18.182	136.424	5.914
Hg	29.944	7.623	12.941
Tl	31.521	26.464	5.429
Pb	32.079	39.787	4.403
Bi	36.985	42.539	4.550
Po	37.534	45.385	4.633
Rn	93.106	0.553	7.240