VASP2012/VASP

VASP 2012 PAW dataset / VASP 5.2.12

`name and version of the code:` VASP 5.2.12
`type of basis set:` plane waves
`method:` projector-augmented wave (VASP 2012)

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_h 06Feb2004	1	900	15 × 15 × 11
He	PAW_PBE He 05Jan2001	2	600	21 × 21 × 11
Li*	PAW_PBE Li_sv 10Sep2004	3	700	15 × 15 × 15
Be	PAW_PBE Be 06Sep2000	2	400	21 × 21 × 11
B*	PAW_PBE B 06Sep2000	3	600	13 × 13 × 13
C	PAW_PBE C 08Apr2002	4	600	17 × 17 × 9
N	PAW_PBE N_h 06Feb2004	5	900	11 × 11 × 11
O	PAW_PBE O_h 06Feb2004	6	900	15 × 15 × 13
F	PAW_PBE F_h 06Feb2004	7	900	9 × 13 × 7
Ne	PAW_PBE Ne 05Jan2001	8	600	13 × 13 × 13
Na*	PAW_PBE Na_pv 19Sep2006	7	400	15 × 15 × 15
Mg	PAW_PBE Mg 13Apr2007	2	400	21 × 21 × 11
Al	PAW_PBE Al 04Jan2001	3	400	13 × 13 × 13
Si*	PAW_PBE Si_h 04Apr2014	4	600	15 × 15 × 15
P	PAW_PBE P_h 08Apr2002	5	600	15 × 5 × 11
S	PAW_PBE S_h 08Apr2002	6	600	19 × 19 × 19
Cl	PAW_PBE Cl_h 21Jan2003	7	600	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_sv 06Sep2000	10	400	13 × 13 × 13
Sc	PAW_PBE Sc_sv 07Sep2000	11	400	21 × 21 × 11
Ti	PAW_PBE Ti_sv 26Sep2005	12	400	21 × 21 × 11
V	PAW_PBE V_sv 02Aug2007	13	400	15 × 15 × 15
Cr	PAW_PBE Cr_pv 02Aug2007	12	400	15 × 15 × 15
Mn	PAW_PBE Mn_pv 02Aug2007	13	400	13 × 13 × 13
Fe	PAW_PBE Fe 06Sep2000	8	400	15 × 15 × 15
Co	PAW_PBE Co 02Aug2007	9	400	21 × 21 × 11
Ni	PAW_PBE Ni 02Aug2007	10	400	13 × 13 × 13
Cu	PAW_PBE Cu 22Jun2005	11	400	13 × 13 × 13
Zn	PAW_PBE Zn 06Sep2000	12	400	21 × 21 × 11
Ga	PAW_PBE Ga_d 06Jul2010	13	400	11 × 11 × 11
Ge*	PAW_PBE Ge_d 03Jul2007	14	400	15 × 15 × 15
As	PAW_PBE As 22Sep2009	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 25May2007	11	400	21 × 21 × 11
Zr	PAW_PBE Zr_sv 04Jan2005	12	400	21 × 21 × 11
Nb	PAW_PBE Nb_sv 25May2007	13	400	15 × 15 × 15
Mo	PAW_PBE Mo_sv 02Feb2006	14	400	15 × 15 × 15
Tc	PAW_PBE Tc_pv 04Feb2005	13	400	21 × 21 × 11
Ru	PAW_PBE Ru_pv 28Jan2005	14	400	21 × 21 × 11
Rh	PAW_PBE Rh_pv 25Jan2005	15	400	13 × 13 × 13
Pd	PAW_PBE Pd 04Jan2005	10	400	13 × 13 × 13
Ag	PAW_PBE Ag 02Apr2005	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 × 15
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 06Nov2007	12	400	15 × 15 × 15
Re	PAW_PBE Re 17Jan2003	7	400	21 × 21 × 11
Os	PAW_PBE Os 17Jan2003	8	400	21 × 21 × 11
Ir	PAW_PBE Ir 06Sep2000	9	400	13 × 13 × 13
Pt	PAW_PBE Pt 04Feb2005	10	400	13 × 13 × 13
Au	PAW_PBE Au 04Oct2007	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	17.411	10.313	2.703
He	17.721	0.922	7.423
Li	20.238	13.820	3.663
Be	7.918	123.340	3.293
B	7.247	237.345	3.475
C	11.660	208.499	3.558
N	28.839	54.099	3.692
O	18.523	51.113	3.916
F	19.176	34.576	4.166
Ne	24.604	1.071	14.688
Na	37.043	7.687	2.993
Mg	22.867	36.579	3.921
Al	16.487	77.293	4.653
Si	20.444	88.606	4.274
P	21.413	68.312	4.349
S	17.189	83.514	4.062
Cl	38.554	19.078	4.387
Ar	52.635	0.789	7.351
K	73.789	3.600	3.850
Ca	42.322	17.388	2.944
Sc	24.657	54.410	3.404
Ti	17.360	111.491	3.686
V	13.476	181.679	4.082
Cr	11.756	180.144	7.166
Mn	11.459	110.946	−0.051
Fe	11.353	186.831	4.924
Co	10.821	209.710	4.534
Ni	10.885	195.436	4.842
Cu	12.011	137.416	4.896
Zn	15.252	74.387	5.639
Ga	20.374	48.662	5.082
Ge	23.888	58.754	4.831
As	22.671	68.755	4.299
Se	29.806	47.268	4.481
Br	39.432	22.480	4.847
Kr	66.507	0.681	4.840
Rb	91.088	2.793	3.799
Sr	54.553	11.106	4.159
Y	32.781	41.204	3.123
Zr	23.408	93.545	3.475
Nb	18.117	170.563	4.051
Mo	15.829	259.543	4.197
Tc	14.415	300.268	4.504
Ru	13.767	313.047	4.901
Rh	14.053	256.275	5.185
Pd	15.295	169.058	5.594
Ag	17.836	90.687	5.765
Cd	22.956	43.620	6.994
In	27.506	35.211	5.364

Sn	36.824	35.751	4.814
Sb	31.766	50.927	4.546
Te	34.961	44.960	4.717
I	50.123	18.720	5.090
Xe	87.660	0.526	7.830
Cs	116.955	1.974	3.488
Ba	63.587	8.864	3.126
Lu	29.389	47.256	3.443
Hf	22.448	108.212	3.420
Ta	18.295	194.986	3.849
W	16.152	305.640	4.265
Re	14.932	372.367	4.540
Os	14.272	405.451	4.957
Ir	14.518	349.151	5.180
Pt	15.613	249.470	5.505
Au	17.959	139.237	5.869
Hg	30.074	6.845	13.752
Tl	31.429	26.514	5.355
Pb	31.994	39.897	4.733
Bi	36.892	42.635	4.555
Po	37.535	45.373	4.639
Rn	93.079	0.553	7.260