VASPGW2015/VASP

VASP 5.4 2015 GW-ready 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 5.4 2015 GW-ready)

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

Aspherical contributions from the gradient corrections inside the PAW spheres have been included.

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 H_h_GW 21Apr2008	1	900	15 × 15 × 11
He	PAW He_GW 13May2007	2	600	21 × 21 × 11
Li*	PAW Li_sv_GW 25Mar2010	3	600	15 × 15 × 15
Be	PAW Be_sv_GW 31Mar2010	4	700	21 × 21 × 11
B*	PAW B_GW 28Sep2005	3	600	13 × 13 × 13
C	PAW C_GW 28Sep2005	4	600	17 × 17 × 9
N	PAW_PBE N_h_GW 03Jul2013	5	1200	11 × 11 × 11
O	PAW_PBE O_h_GW 22May2013	6	1200	15 × 15 × 13
F	PAW_PBE F_h_GW 03Jul2013	7	1300	9 × 13 × 7
Ne	PAW_PBE Ne_GW 21Aug2013	8	500	13 × 13 × 13
Na*	PAW_PBE Na_sv_GW 11May2015	9	600	15 × 15 × 15
Mg	PAW Mg_sv_GW 20Apr2010	10	600	21 × 21 × 11
Al	PAW Al_GW 19Mar2012	3	400	13 × 13 × 13
Si*	PAW Si_GW 04May2012	4	400	15 × 15 × 15
P	PAW P_GW 19Mar2012	5	400	15 × 5 × 11
S	PAW S_GW 19Mar2012	6	400	19 × 19 × 19
Cl	PAW Cl_GW 19Mar2012	7	400	13 × 13 × 13
Ar	PAW_PBE Ar_GW 21Aug2013	8	400	13 × 13 × 13
K	PAW K_sv_GW 31Mar2010	9	400	15 × 15 × 15
Ca	PAW Ca_sv_GW 31Mar2010	10	400	13 × 13 × 13
Sc	PAW Sc_sv_GW 05Dec2013	11	400	21 × 21 × 11
Ti	PAW Ti_sv_GW 05Dec2013	12	400	21 × 21 × 11
V	PAW V_sv_GW 05Dec2013	13	500	15 × 15 × 15
Cr	PAW Cr_sv_GW 05Dec2013	14	500	15 × 15 × 15
Mn	PAW Mn_sv_GW 05Dec2013	15	500	13 × 13 × 13
Fe	PAW Fe_sv_GW 05Dec2013	16	500	15 × 15 × 15
Co	PAW Co_sv_GW 05Dec2013	17	500	21 × 21 × 11
Ni	PAW Ni_sv_GW 05Dec2013	18	500	13 × 13 × 13
Cu	PAW Cu_sv_GW 10Dec2015	11	700	13 × 13 × 13
Zn	PAW Zn_sv_GW 05Dec2013	12	600	21 × 21 × 11
Ga	PAW Ga_d_GW 15Mar2013	13	600	11 × 11 × 11
Ge*	PAW Ge_d_GW 19Mar2013	14	400	15 × 15 × 15
As	PAW As_GW 20Mar2012	5	400	17 × 17 × 7
Se	PAW Se_GW 20Mar2012	6	400	13 × 13 × 13
Br	PAW_PBE Br_GW 20Mar2012	7	400	13 × 13 × 13
Kr	PAW_PBE Kr_GW 21Aug2013	8	400	13 × 13 × 13
Rb	PAW Rb_sv_GW 23Mar2010	9	400	15 × 15 × 15
Sr	PAW Sr_sv_GW 23Mar2010	10	400	15 × 15 × 15
Y	PAW Y_sv_GW 05Dec2013	11	400	21 × 21 × 11
Zr	PAW Zr_sv_GW 05Dec2013	12	400	21 × 21 × 11
Nb	PAW Nb_sv_GW 05Dec2013	13	400	15 × 15 × 15
Mo	PAW Mo_sv_GW 05Dec2013	14	400	15 × 15 × 15
Tc	PAW Tc_sv_GW 05Dec2013	15	500	21 × 21 × 11
Ru	PAW Ru_sv_GW 05Dec2013	16	500	21 × 21 × 11
Rh	PAW Rh_sv_GW 05Dec2013	17	500	13 × 13 × 13
Pd	PAW Pd_sv_GW 05Dec2013	18	500	13 × 13 × 13
Ag	PAW Ag_sv_GW 05Dec2013	19	500	13 × 13 × 13
Cd	PAW Cd_sv_GW 22Nov2013	20	500	21 × 21 × 11

In	PAW In_d_GW 15Mar2013	13	400	19 × 19 × 15
Sn*	PAW_PBE Sn_d_GW 15Mar2013	14	400	15 × 15 × 15
Sb	PAW Sb_d_GW 15Mar2013	15	400	17 × 17 × 7
Te	PAW Te_GW 22Mar2012	6	400	13 × 13 × 13
I	PAW_PBE I_GW 12Mar2012	7	400	13 × 13 × 13
Xe	PAW Xe_GW 08Jan2009	8	400	13 × 13 × 13
Cs	PAW Cs_sv_GW 23Mar2010	9	400	15 × 15 × 15
Ba	PAW Ba_sv_GW 23Mar2010	10	400	15 × 15 × 15
Lu	*N/A*	*N/A*	*N/A*	*N/A*
Hf	PAW Hf_sv_GW 05Jan2015	12	400	21 × 21 × 11
Ta	PAW Ta_sv_GW 23Mar2010	13	400	15 × 15 × 15
W	PAW W_sv_GW 23Mar2010	14	500	15 × 15 × 15
Re	PAW Re_sv_GW 23Mar2010	15	500	21 × 21 × 11
Os	PAW Os_sv_GW 23Mar2010	16	500	21 × 21 × 11
Ir	PAW Ir_sv_GW 23Mar2010	17	500	13 × 13 × 13
Pt	PAW Pt_sv_GW 23Mar2010	18	500	13 × 13 × 13
Au	PAW Au_sv_GW 13Sep2013	19	500	13 × 13 × 13
Hg	*N/A*	*N/A*	*N/A*	*N/A*
Tl	*N/A*	*N/A*	*N/A*	*N/A*
Pb	PAW Pb_d 06Oct2005	14	400	13 × 13 × 13
Bi	PAW_PBE Bi_d_GW 22Jun2012	15	400	17 × 17 × 7
Po	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*

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	17.408	10.304	2.709
He	17.860	0.833	6.602
Li	20.200	13.685	3.607
Be	7.889	124.461	3.512
B	7.237	237.067	3.470
C	11.631	208.827	3.566
N	28.823	53.953	3.688
O	18.553	50.827	3.839
F	19.152	34.335	4.081
Ne	24.837	1.042	11.848
Na	37.228	7.701	3.824
Mg	22.929	35.978	4.171
Al	16.463	77.705	4.639
Si	20.460	88.753	4.297
P	21.469	68.019	4.332
S	17.197	83.516	4.122
Cl	38.885	18.919	4.392
Ar	52.808	0.759	7.016
K	73.554	3.617	4.034
Ca	42.097	17.361	3.283
Sc	24.594	54.028	3.248
Ti	17.404	112.362	3.350
V	13.452	182.503	4.006
Cr	11.792	185.194	6.902
Mn	11.450	118.394	−0.420
Fe	11.344	198.092	4.936
Co	10.856	215.805	4.676
Ni	10.903	200.339	5.190
Cu	11.946	141.246	4.665
Zn	15.218	74.858	5.134
Ga	20.380	48.679	5.297
Ge	23.972	58.134	4.914
As	22.640	68.880	4.301
Se	29.779	47.281	4.477
Br	39.408	22.478	4.843
Kr	66.060	0.687	6.131
Rb	91.022	2.803	3.800
Sr	54.602	11.214	3.356
Y	32.892	39.076	−0.220
Zr	23.401	93.901	3.469
Nb	18.138	169.124	3.898
Mo	15.802	259.889	4.225
Tc	14.436	297.758	4.523
Ru	13.759	312.769	4.953
Rh	14.033	258.072	5.512
Pd	15.298	169.795	5.717
Ag	17.831	91.103	5.782
Cd	22.872	42.435	6.720
In	27.445	35.386	5.301

Sn	36.793	35.820	4.834
Sb	31.748	50.474	4.437
Te	34.879	45.036	4.719
I	50.014	18.760	5.082
Xe	87.080	0.530	8.485
Cs	116.910	1.953	3.351
Ba	63.303	8.859	2.959
Lu	*N/A*	*N/A*	*N/A*
Hf	22.493	108.685	3.382
Ta	18.267	194.813	3.835
W	16.122	304.961	4.169
Re	14.946	365.437	4.564
Os	14.285	399.358	4.884
Ir	14.489	348.745	5.221
Pt	15.636	248.407	5.473
Au	17.977	139.248	5.893
Hg	*N/A*	*N/A*	*N/A*
Tl	*N/A*	*N/A*	*N/A*
Pb	32.008	39.910	4.738
Bi	36.851	42.590	4.566
Po	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*