

VASPGW2012/VASP

VASP 5.2 2012 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 5.2 2012 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 $2G_{cut} = 2\sqrt{\frac{2m_e E_{cut}}{\hbar^2}}$ included
augmentation charge grid	wavevectors up to $4G_{cut}$ 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).

VASPGW2012/VASP

VASP 5.2 2012 GW-ready PAW dataset / VASP 5.2.12

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 N.GW 10Apr2007	5	600	11 × 11 × 11
O	PAW O.GW 28Sep2005	6	600	15 × 15 × 13
F	PAW F.GW 21Dec2007	7	700	9 × 13 × 7
Ne	PAW Ne.GW 02Oct2006	8	500	13 × 13 × 13
Na*	PAW Na_sv.GW 08Feb2008	9	400	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 Ar.GW 02Oct2006	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 23Mar2010	11	400	21 × 21 × 11
Ti	PAW Ti_sv.GW 23Mar2010	12	400	21 × 21 × 11
V	PAW V_sv.GW 31Mar2010	13	500	15 × 15 × 15
Cr	PAW Cr_sv.GW 31Mar2010	14	500	15 × 15 × 15
Mn	PAW Mn_sv.GW 27Nov2009	15	500	13 × 13 × 13
Fe	PAW Fe_sv.GW 31Mar2010	16	500	15 × 15 × 15
Co	PAW Co_sv.GW 27Nov2009	17	500	21 × 21 × 11
Ni	PAW Ni_sv.GW 27Nov2009	18	600	13 × 13 × 13
Cu	PAW Cu.GW 19May2006	11	600	13 × 13 × 13
Zn	PAW Zn.GW 09Oct2010	12	500	21 × 21 × 11
Ga	PAW Ga_d.GW 06Jul2010	13	600	11 × 11 × 11
Ge*	PAW Ge_d.GW 17Dec2007	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 Kr.GW 02Oct2006	8	400	13 × 13 × 13
Rb	PAW Rb_sv.GW 23Mar2010	9	400	15 × 15 × 15
Sr	PAW Sr_sv.GW 23Mar2010	10	400	13 × 13 × 13
Y	PAW Y_sv.GW 23Mar2010	11	400	21 × 21 × 11
Zr	PAW Zr_sv.GW 07Apr2010	12	400	21 × 21 × 11
Nb	PAW Nb_sv.GW 23Mar2010	13	400	15 × 15 × 15
Mo	PAW Mo_sv.GW 23Mar2010	14	400	15 × 15 × 15
Tc	PAW Tc_sv.GW 23Mar2010	15	500	21 × 21 × 11
Ru	PAW Ru_sv.GW 23Mar2010	16	500	21 × 21 × 11
Rh	PAW Rh_sv.GW 20Mar2012	17	500	13 × 13 × 13
Pd	PAW Pd.GW 06Mar2008	10	400	13 × 13 × 13
Ag	PAW Ag.GW 06Mar2008	11	400	13 × 13 × 13
Cd	PAW Cd.GW 18May2010	12	400	21 × 21 × 11

VASPGW2012/VASP

VASP 5.2 2012 GW-ready PAW dataset / VASP 5.2.12

In	PAW In_d_GW 29May2007	13	400	19 × 19 × 15
Sn*	PAW_PBE Sn_d_GW 20Mar2012	14	400	15 × 15 × 15
Sb	PAW Sb_GW 21Mar2012	5	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	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Hf	PAW Hf_sv_GW 25Mar2010	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_GW 10Mar2009	10	400	13 × 13 × 13
Au	PAW Au_GW 23Mar2010	11	400	13 × 13 × 13
Hg	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Tl	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Pb	PAW Pb_d 06Oct2005	14	400	13 × 13 × 13
Bi	PAW_PBE Bi_d_GW 22Apr2009	15	400	17 × 17 × 7
Po	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Rn	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>

VASPGW2012/VASP

VASP 5.2 2012 GW-ready PAW dataset / VASP 5.2.12

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 [$\text{\AA}^3/\text{atom}$]	B_0 [GPa]	B_1 [-]
H	17.410	10.301	2.710
He	17.860	0.833	6.602
Li	20.200	13.685	3.607
Be	7.889	124.457	3.512
B	7.237	237.033	3.470
C	11.635	208.766	3.565
N	29.174	54.877	3.782
O	18.903	51.510	4.017
F	19.379	34.283	4.092
Ne	24.336	1.518	12.082
Na	37.255	7.685	3.131
Mg	22.929	35.978	4.171
Al	16.463	77.705	4.639
Si	20.458	88.787	4.320
P	21.465	68.001	4.334
S	17.198	83.522	4.121
Cl	38.854	18.969	4.398
Ar	52.723	0.778	7.258
K	73.554	3.617	4.034
Ca	42.097	17.361	3.283
Sc	24.617	54.852	3.394
Ti	17.401	111.057	3.554
V	13.373	193.664	10.314
Cr	11.757	185.518	6.909
Mn	11.355	108.356	0.582
Fe	11.364	192.509	4.651
Co	10.837	212.112	4.652
Ni	10.843	199.223	4.691
Cu	11.966	138.686	4.994
Zn	15.222	74.620	5.167
Ga	20.371	48.670	5.305
Ge	23.909	58.643	4.897
As	22.642	68.877	4.302
Se	29.773	47.334	4.480
Br	39.375	22.527	4.848
Kr	66.106	0.682	5.890
Rb	91.022	2.803	3.800
Sr	54.583	10.784	5.352
Y	32.909	41.242	3.157
Zr	23.426	93.473	3.441
Nb	18.161	169.747	4.064
Mo	15.817	259.768	4.226
Tc	14.444	299.304	4.543
Ru	13.767	312.941	4.913
Rh	14.071	257.145	5.391
Pd	15.231	169.915	5.565
Ag	17.817	91.009	5.763
Cd	22.802	44.192	6.952
In	27.460	35.262	5.321

VASPGW2012/VASP

VASP 5.2 2012 GW-ready PAW dataset / VASP 5.2.12

Sn	36.783	35.747	4.941
Sb	31.687	51.065	4.555
Te	34.877	45.044	4.719
I	49.991	18.780	5.086
Xe	87.080	0.530	8.485
Cs	116.910	1.953	3.351
Ba	63.304	8.859	2.955
Lu	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Hf	22.462	108.465	3.398
Ta	18.267	194.814	3.831
W	16.122	304.968	4.171
Re	14.946	365.438	4.565
Os	14.285	399.357	4.884
Ir	14.489	348.758	5.224
Pt	15.587	250.461	5.521
Au	17.937	139.943	5.843
Hg	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Tl	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Pb	32.008	39.910	4.738
Bi	36.864	42.596	4.519
Po	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>
Rn	<i>N/A</i>	<i>N/A</i>	<i>N/A</i>