GPAW06(g)/GPAW

GPAW 0.6 PAW dataset / GPAW 0.8.0 grid-based

`name and version of the code:` GPAW 0.8.0
`type of basis set:` grid-based
`method:` projector-augmented wave (GPAW 0.6)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table (Z_{val})
`basis set size`	real-space grid spacing = 0.075 Å
`k-mesh density`	see table (k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts*, and number of irreducible k-points # *k*)
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.1 eV

METHOD-SPECIFIC INFORMATION

none

ADDITIONAL COMMENTS

none

REFERENCES

`PAW dataset`

[1] https://wiki.fysik.dtu.dk/gpaw/setups/setups.html

`code`

[2] J. J. Mortensen, L. B. Hansen, K. W. Jacobsen, *Phys. Rev. B* **71**, 035109 (2005).
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`scalar relativity`

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

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Table I. Calculation settings and results per element: valence Z_{val}, k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts* and number of irreducible k-points # k, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	Z_{val} [–]	*kpts* [–]	# k [–]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	1	15 × 15 × 11	257	17.465	10.332	2.932
He	2	21 × 21 × 11	288	17.693	0.841	6.728
Li	1	15 × 15 × 15	344	20.278	14.028	3.412
Be	2	21 × 21 × 11	288	8.009	123.338	3.371
B	3	13 × 13 × 13	231	7.242	237.135	3.527
C	4	17 × 17 × 9	261	11.648	208.653	3.623
N	5	11 × 11 × 11	226	28.910	54.005	3.666
O	6	15 × 15 × 13	784	19.280	53.607	3.964
F	7	17 × 17 × 7	1 012	19.207	33.730	4.501
Ne	8	13 × 13 × 13	84	23.751	2.057	20.674
Na	1	15 × 15 × 15	344	37.045	7.814	3.913
Mg	2	21 × 21 × 11	288	22.971	36.255	4.182
Al	3	13 × 13 × 13	84	16.515	78.209	4.610
Si	4	15 × 15 × 15	120	20.521	88.830	4.361
P	5	15 × 5 × 11	224	21.531	68.072	4.436
S	6	19 × 19 × 19	670	17.224	83.735	4.316
Cl	7	13 × 13 × 13	595	38.953	19.016	4.590
Ar	8	13 × 13 × 13	84	52.661	0.838	3.274
K	9	15 × 15 × 15	120	73.782	3.605	2.491
Ca	10	13 × 13 × 13	84	42.456	17.399	3.193
Sc	11	21 × 21 × 11	288	24.670	53.839	2.540
Ti	12	21 × 21 × 11	288	17.257	114.395	3.714
V	5	15 × 15 × 15	120	13.729	185.469	4.379
Cr	6	15 × 15 × 15	120	11.870	161.790	6.665
Mn	7	13 × 13 × 13	196	11.746	126.641	1.116
Fe	8	15 × 15 × 15	120	11.478	196.731	5.034
Co	9	21 × 21 × 11	288	10.921	212.449	4.997
Ni	10	13 × 13 × 13	84	10.917	203.624	4.602
Cu	11	13 × 13 × 13	84	12.100	139.364	4.594
Zn	12	21 × 21 × 11	288	15.250	75.075	4.797
Ga	3	13 × 13 × 11	504	20.524	50.277	5.242
Ge	4	15 × 15 × 15	120	23.979	60.055	4.840
As	5	17 × 17 × 7	204	22.636	68.863	4.434
Se	6	13 × 13 × 13	595	29.749	47.176	4.607
Br	7	13 × 13 × 13	595	40.382	20.802	4.658
Kr	8	13 × 13 × 13	84	65.583	0.807	13.160
Rb	9	15 × 15 × 15	120	91.172	2.694	3.056
Sr	10	13 × 13 × 13	84	55.154	11.183	3.684
Y	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Zr	12	21 × 21 × 11	288	23.458	94.850	3.384
Nb	5	15 × 15 × 15	120	18.232	174.183	3.783
Mo	6	15 × 15 × 15	120	15.888	263.725	4.375
Tc	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Ru	8	21 × 21 × 11	288	14.090	310.945	4.874
Rh	9	13 × 13 × 13	84	14.321	255.152	5.424
Pd	10	13 × 13 × 13	84	15.415	167.311	5.975
Ag	11	13 × 13 × 13	84	18.067	90.687	5.520
Cd	12	21 × 21 × 11	288	22.875	43.266	6.282

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In	13	19 × 19 × 15	440	27.533	35.147	5.603
Sn	14	15 × 15 × 15	120	36.899	35.991	4.899
Sb	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Te	16	13 × 13 × 13	595	34.171	46.105	4.812
I	7	13 × 13 × 13	595	51.154	17.551	4.878
Xe	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Cs	9	15 × 15 × 15	120	117.011	2.115	3.588
Ba	10	15 × 15 × 15	120	63.514	8.930	2.947
Lu	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Hf	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Ta	5	15 × 15 × 15	120	18.523	198.352	3.991
W	6	15 × 15 × 15	120	16.440	307.490	4.351
Re	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Os	8	21 × 21 × 11	288	14.517	397.939	4.975
Ir	9	13 × 13 × 13	84	14.699	351.625	5.385
Pt	10	13 × 13 × 13	84	15.790	247.633	5.666
Au	11	13 × 13 × 13	84	18.207	137.822	5.772
Hg	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Tl	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Pb	14	13 × 13 × 13	84	32.103	39.060	5.556
Bi	15	17 × 17 × 7	204	36.973	42.857	4.761
Po	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*
Rn	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*	*N/A*