`name and version of the code:` ABINIT 7.8.2
`type of basis set:` plane waves
`method:` projector-augmented wave (JTH 1.0)

GENERAL INFORMATION

`exchange-correlation functional`	PBE
`relativistic scheme`	core and valence scalar relativistic (Koelling-Harmon)
`assignment of core / valence states`	see table
`basis set size`	cutoff energy $= 20\,\mathrm{Ha}$
`k-mesh density`	$6\,750/N$ k-points in the full first Brillouin zone of an N-atom cell
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to $0.002\,\mathrm{Ha}$

METHOD-SPECIFIC INFORMATION

`PAW radii`	see table (R_{PAW})
`PAW cutoff energy`	$20\,\mathrm{Ha}$
`PAW cutoff augmentation energy`	$40\,\mathrm{Ha}$
`Partial-wave basis size`	2 elements per ℓ-value except Li (three s elements), H, He (one p element) and K, Kr, Rb (one d element)

ADDITIONAL COMMENTS

`PAW dataset generator`	ATOMPAW 4.0.0.12

REFERENCES

`PAW dataset`

[1] http://pwpaw.wfu.edu
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[3] F. Jollet, M. Torrent and N. Holzwarth, *Comput. Phys. Commun.* **185**, 1246–1254 (2014).

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[6] M. Torrent, F. Jollet, F. Bottin, G. Zérah, X. Gonze, *Comput. Mater. Sci.* **42**, 337–351, (2008).

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

Table I. Calculation settings and results per element: valence, PAW radius R_{PAW}, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	valence	R_{PAW} [a.u.]	V_0 [Å³/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1\ 2p^0$	0.9	17.49784	10.19793	3.158
He	$1s^2\ 2p^0$	1.3	17.82456	0.83536	6.413
Li	$1s^2\ 2s^1\ 2p^0$	1.6	20.21678	13.93010	3.312
Be	$1s^2\ 2s^2$	1.6	7.90653	122.83641	2.998
B	$2s^2\ 2p^1$	1.7	7.24518	237.25091	3.487
C	$2s^2\ 2p^2$	1.5	11.63849	211.23278	2.774
N	$2s^2\ 2p^3$	1.2	28.92990	55.15457	3.028
O	$2s^2\ 2p^4$	1.4	18.58062	51.28722	3.909
F	$2s^2\ 2p^5$	1.4	19.18638	35.47908	4.280
Ne	$2s^2\ 2p^6$	1.8	24.26853	1.47723	10.440
Na	$2s^2\ 2p^6\ 3s^1$	1.6	37.15343	7.96188	4.874
Mg	$2s^2\ 2p^6\ 3s^2$	1.9	22.95909	35.68261	5.188
Al	$3s^2\ 3p^1$	1.9	16.47447	77.74370	4.560
Si	$3s^2\ 3p^2$	1.9	20.43663	88.78771	4.362
P	$3s^2\ 3p^3$	1.9	21.43844	67.88073	4.375
S	$3s^2\ 3p^4$	1.9	17.16799	83.68796	4.129
Cl	$3s^2\ 3p^5$	1.8	38.88399	18.80925	4.305
Ar	$3s^2\ 3p^6$	1.8	52.70597	0.77477	−8.589
K	$3s^2\ 3p^6\ 4s^1\ 3d^0$	2.1	73.78410	3.62429	3.657
Ca	$3s^2\ 3p^6\ 4s^2\ 3d^0$	1.9	42.15503	17.36928	4.457
Sc	$3s^2\ 3p^6\ 4s^2\ 3d^1$	2.4	24.62132	54.28819	3.379
Ti	$3s^2\ 3p^6\ 4s^1\ 3d^3$	2.3	17.44179	111.26898	3.586
V	$3s^2\ 3p^6\ 4s^2\ 3d^3$	2.2	13.49462	180.72451	3.812
Cr	$3s^2\ 3p^6\ 4s^1\ 3d^5$	2.1	11.76507	176.02398	6.499
Mn	$3s^2\ 3p^6\ 4s^1\ 3d^6$	2.1	11.46933	109.23894	1.795
Fe	$3s^2\ 3p^6\ 4s^1\ 3d^7$	2.1	11.35042	188.26412	4.337
Co	$3s^2\ 3p^6\ 4s^1\ 3d^8$	2.1	10.88408	212.91538	5.008
Ni	$3s^2\ 3p^6\ 4s^2\ 3d^8$	1.8	10.92726	195.27345	4.504
Cu	$3s^2\ 3p^6\ 4s^1\ 3d^{10}$	2.0	11.98367	143.88972	3.113
Zn	$4s^2\ 4p^0\ 3d^{10}$	2.3	15.17410	75.61000	5.861
Ga	$4s^2\ 4p^1\ 3d^{10}$	2.1	20.32112	49.24926	5.152
Ge	$4s^2\ 4p^2\ 3d^{10}$	2.3	23.95958	58.74576	4.844
As	$4s^2\ 4p^3\ 3d^{10}$	2.1	22.62153	68.42866	4.256
Se	$4s^2\ 4p^4$	2.2	29.76678	47.18222	4.410
Br	$4s^2\ 4p^5$	2.2	39.42359	22.42968	4.955
Kr	$4s^2\ 4p^6\ 4d^0$	2.2	65.58856	0.66720	7.045
Rb	$4s^2\ 4p^6\ 5s^1\ 4d^0$	2.3	91.35346	2.76524	3.710
Sr	$4s^2\ 4p^6\ 5s^1\ 4d^1$	2.2	54.81820	11.66688	3.546
Y	$4s^2\ 4p^6\ 5s^2\ 4d^1$	2.21	32.87962	40.84878	3.090
Zr	$4s^2\ 4p^6\ 5s^1\ 4d^3$	2.21	23.39635	93.35861	3.307
Nb	$4s^2\ 4p^6\ 5s^1\ 4d^4$	2.21	18.13476	169.28294	3.675
Mo	$4s^2\ 4p^6\ 5s^1\ 4d^5$	2.2	15.81546	259.32212	4.228
Tc	$4s^2\ 4p^6\ 5s^1\ 4d^6$	2.2	14.42049	300.50292	4.496
Ru	$4s^2\ 4p^6\ 5s^1\ 4d^7$	2.2	13.75825	310.20598	4.882
Rh	$4s^2\ 4p^6\ 5s^1\ 4d^8$	2.4	14.02331	259.21608	5.199
Pd	$4s^2\ 4p^6\ 5s^1\ 4d^9$	2.5	15.34098	165.54672	5.834
Ag	$5s^1\ 5p^0\ 4d^{10}$	2.5	17.83568	92.00123	5.850
Cd	$5s^2\ 5p^0\ 4d^{9.5}$	2.5	22.83952	43.96281	6.457
In	$5s^2\ 5p^1\ 4d^{10}$	2.5	27.44337	36.31721	6.098

Sn	$5s^2\ 5p^2\ 4d^{10}$	2.5	36.81800	36.04592	5.462
Sb	$5s^2\ 5p^3\ 4d^{10}$	2.4	31.75873	50.35566	4.390
Te	$5s^2\ 5p^4$	2.3	34.97177	45.14244	4.735
I	$5s^2\ 5p^5$	2.3	50.40996	18.73037	5.018
Xe	$5s^2\ 5p^6$	2.4	86.82364	0.53258	3.803
Cs	$5s^2\ 5p^6\ 6s^1\ 5d^0$	2.2	117.24092	1.95497	4.664
Ba	$5s^2\ 5p^6\ 6s^2\ 5d^0$	2.3	63.48759	8.49481	5.911
Lu	$5s^2\ 5p^6\ 6s^2\ 5d^1\ 4f^{14}$	2.5	29.05320	47.69130	3.517
Hf	$5s^2\ 5p^6\ 6s^2\ 5d^2$	2.41	22.54152	107.55827	3.302
Ta	$5s^2\ 5p^6\ 6s^2\ 5d^3$	2.41	18.29414	198.35505	3.400
W	$5s^2\ 5p^6\ 6s^2\ 5d^4$	2.41	16.16008	303.53815	4.137
Re	$5s^2\ 5p^6\ 6s^2\ 5d^5$	2.4	14.96913	365.51908	4.377
Os	$5p^6\ 6s^1\ 5d^7$	2.5	14.28354	402.30170	4.747
Ir	$5p^6\ 6s^1\ 5d^8$	2.5	14.49380	351.29775	5.199
Pt	$6s^1\ 6p^0\ 5d^9$	2.5	15.67922	250.16206	5.560
Au	$6s^1\ 6p^0\ 5d^{10}$	2.5	18.01120	140.30086	5.501
Hg	$6s^2\ 6p^0\ 5d^{10}$	2.4	29.54526	9.07820	12.115
Tl	$6s^2\ 6p^1\ 5d^{10}$	2.4	31.38576	26.60783	5.434
Pb	$6s^2\ 6p^2\ 5d^{10}$	2.4	32.02278	40.07972	5.365
Bi	$6s^2\ 6p^3\ 5d^{10}$	2.4	36.89370	42.61470	4.651
Po	$6s^2\ 6p^4$	2.9	37.57022	46.08312	4.848
Rn	$6s^2\ 6p^6$	2.3	92.99970	0.54887	4.831