ELEMENTAL BULKS

Z	Element	Material ID	Space Group	Crystal System	Lattice constant (Å)	Bulk Modulus (GPa)	Bandgap (eV)	Ecut (eV)	K-points
3	Li	mp-135	Im-3m	bcc	3.439	14.23	0.0	525.0	16, 16, 16 (4.7)
4	Be	mp-87	P6_3/mmc	hexagonal	2.263, 3.575	124.85	/	300.0	15 15 9 (4.6)
6	C	mp-66	Fd-3m	fcc	3.573	430.29	4.097	400.0	12, 12, 12 (3.3)
11	Na	mp-127	Im-3m	bcc	4.193	7.98	0.0	300.0	22, 22, 22 (5.2)
12	Mg	mp-153	P6_3/mmc	hexagonal	3.208, 5.135	35.66	0.0	400.0	15 15 8 (6.2)
13	Al	mp-134	Fm-3m	fcc	4.045	76.93	0.0	275.0	26, 26, 26 (6.4)
14	Si	mp-149	Fm-3m	fcc	5.473	87.66	0.659	225.0	20, 20, 20 (3.6)
19	K	mp-58	Im-3m	bcc	5.281	3.48	/	275.0	29, 29, 29 (5.4)
20	Ca	mp-45	Fm-3m	fcc	5.533	17.31	0.0	300.0	20, 20, 20 (3.6)
21	Sc	mp-67	P6_3/mmc	hexagonal	3.319, 5.178	53.49	/	250.0	9 9 5 (3.7)
22	Ti	mp-46	P6_3/mmc	hexagonal	2.935, 4.659	112.17	0.0	250.0	9 9 5 (3.3)
23	V	mp-146	Im-3m	bcc	2.998	181.76	0.0	300.0	15, 15, 15 (5.1)
24	Cr	mp-90	Im-3m	bcc	3.309	179.08	0.0	300.0	12, 12, 12 (3.7)
25	Mn	mp-35	I-43m	cubic	3.309	275.36	/	350.0	5 5 5 (3.9)
26	Fe	mp-13	Im-3m	bcc	2.831	178.45	0.0	325.0	11, 11, 11 (3.9)
27	Co	mp-54	P6_3/mmc	hexagonal	2.492, 4.02	211.62	/	300.0	11 11 6 (3.5)
28	Ni	mp-23	Fm-3m	fcc	3.521	197.37	0.0	400.0	12, 12, 12 (3.3)
29	Cu	mp-30	Fm-3m	fcc	3.633	140.07	0.0	375.0	13, 13, 13 (3.7)
30	Zn	mp-79	P6_3/mmc	hexagonal	2.625, 5.203	72.67	0.0	275.0	16 16 7 (5.5)
32	Ge	mp-32	Fd-3m	fcc	5.761	58.65	0.0	275.0	28, 28, 28 (4.8)
37	Rb	mp-70	Im-3m	bcc	5.677	2.86	/	225.0	33, 33, 33 (5.8)
38	Sr	mp-76	Fm-3m	fcc	6.019	11.61	0.094	225.0	27, 27, 27 (4.5)
39	Y	mp-112	P6_3/mmc	hexagonal	3.658, 5.664	40.35	0.0	275.0	11 11 6 (5.1)
40	Zr	mp-131	P6_3/mmc	hexagonal	3.239, 5.172	93.89	0.0	250.0	8 8 5 (3.3)
41	Nb	mp-75	Im-3m	bcc	3.32	173.68	0.0	200.0	18, 18, 18 (5.3)
42	Mo	mp-129	Im-3m	bcc	3.16	257.98	0.0	250.0	18, 18, 18 (5.7)
43	Tc	mp-113	P6_3/mmc	hexagonal	2.75, 4.404	297.99	0.0	275.0	10 10 5 (3.5)
44	Ru	mp-33	P6_3/mmc	hexagonal	2.72, 4.294	310.38	0.0	275.0	14 14 8 (4.9)
45	Rh	mp-74	Fm-3m	fcc	3.83	254.79	0.0	275.0	16, 16, 16 (4.3)
46	Pd	mp-2	Fm-3m	fcc	3.943	163.92	0.0	275.0	19, 19, 19 (4.8)
47	Ag	mp-124	Fm-3m	fcc	4.149	89.27	0.0	300.0	17, 17, 17 (4.2)
48	Cd	mp-94	P6_3/mmc	hexagonal	3.009, 5.944	42.96	0.0	275.0	16 16 7 (6.3)
55	Cs	mp-1	Im-3m	bcc	6.158	2.08	0.0	225.0	39, 39, 39 (6.3)
56	Ba	mp-122	Im-3m	bcc	5.029	8.89	0.0	225.0	23, 23, 23 (4.6)
57	La	mp-26	P6_3/mmc	hexagonal	3.772, 12.067	25.41	0.0	225.0	8 8 3 (3.9)
60	Nd	mp-123	P6_3/mmc	hexagonal	3.708, 11.915	33.85	0.0	225.0	9 9 3 (4.1)
61	Pm	mp-867200	P6_3/mmc	hexagonal	3.675, 11.826	35.5	0.0	175.0	9 9 3 (4.1)

64	Gd	mp-155	P6_3/mmc	hexagonal	3.65, 5.828	34.58	0.0	250.0	7 7 4 (3.1)
65	Tb	mp-18	P6_3/mmc	hexagonal	3.637, 5.658	39.32	0.0	225.0	13 13 8 (6.4)
66	Dy	mp-88	P6_3/mmc	hexagonal	3.624, 5.613	40.7	0.0	225.0	12 12 7 (5.5)
67	Ho	mp-144	P6_3/mmc	hexagonal	3.608, 5.576	42.11	0.0	225.0	12 12 7 (5.5)
68	Er	mp-99	P6_3/mmc	hexagonal	3.587, 5.546	43.82	0.0	225.0	12 12 7 (5.5)
69	Tm	mp-143	P6_3/mmc	hexagonal	3.566, 5.519	45.14	0.0	200.0	9 9 6 (4.4)
70	Yb	mp-162	Fm-3m	fcc	5.418	15.33	0.0	200.0	24, 24, 24 (4.5)
71	Lu	mp-145	P6_3/mmc	hexagonal	3.524, 5.47	47.03	0.0	225.0	10 10 6 (4.4)
72	Hf	mp-103	P6_3/mmc	hexagonal	3.199, 5.076	108.8	0.0	225.0	8 8 4 (3.1)
73	Ta	mp-50	Im-3m	bcc	3.322	194.02	0.0	200.0	19, 19, 19 (5.7)
74	W	mp-91	Im-3m	bcc	3.186	301.55	0.0	225.0	25, 25, 25 (7.9)
75	Re	mp-8	P6_3/mmc	hexagonal	2.777, 4.491	364.4	0.0	275.0	9 9 5 (3.1)
76	Os	mp-49	P6_3/mmc	hexagonal	2.757, 4.354	402.6	0.0	250.0	13 13 8 (4.9)
77	Ir	mp-101	Fm-3m	fcc	3.872	349.0	0.0	225.0	29, 29, 29 (7.5)
78	Pt	mp-126	Fm-3m	fcc	3.968	247.15	0.0	250.0	23, 23, 23 (5.9)
79	Au	mp-81	Fm-3m	fcc	4.158	137.47	0.0	275.0	21, 21, 21 (5)
81	Tl	mp-82	P6_3/mmc	hexagonal	3.55, 5.74	27.0	0.0	250.0	12 12 6 (5.4)
82	Pb	mp-20483	Fm-3m	fcc	5.039	39.81	0.0	250.0	31, 31, 31 (6.1)
89	Ac	mp-10018	Fm-3m	fcc	5.675	23.73	0.0	175.0	24, 24, 24 (4.2)
90	Th	mp-37	Fm-3m	fcc	5.056	55.89	0.0	250.0	45, 45, 45 (8.9)

All the calculations reported in the table have been performed with the Vienna Ab Initio Simulation Package (VASP, https://www.vasp.at), pymatgen (https://pymatgen.org), atomate (https://atomate.org), and the FireWorks high throughput library (https://materialsproject.github.io/fireworks/).

Notes:

[1] Most of the Material IDs correspond to the Materials Project IDs reachable at: https://materialsproject.org/.

[2] For the hexagonal crystal systems the reported lattice constants are a and c, and they have been calculated with a variable-cell relaxation (vc-relax) with the PBE exchange-correlation energy functional.

[3] The bulk moduli have been calculated as the second derivative of the total energy with respect to the lattice constant by fitting the Birch-Murnaghan equation of state.

[4] To determine the optimal kinetic energy cut-off for the wave functions, we evaluated the change in the total energy and the lattice parameter of the minima of different Birch-Murnaghan curves.

[5] For the k-points, the Monkhorst-Pack grid and the k-points density are reported (H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976)).