

Supplementary Materials: The AFLOW Standard for High-Throughput Materials Science Calculations

Camilo E. Calderon¹, Jose J. Plata¹, Cormac Toher¹, Corey Oses¹, Ohad Levy^{1,†},
Marco Fornari², Amir Natan³, Michael J. Mehl⁴, Gus Hart⁵, Marco Buongiorno Nardelli⁶, Stefano Curtarolo^{7,*}

¹*Department of Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina 27708, USA*

²*Department of Physics, Central Michigan University, Mount Pleasant, MI 48858, USA*

³*Department Of Physics And Electrical Engineering & Electronics, Faculty of Engineering, Tel Aviv University, Tel Aviv 69978, Israel*

⁴*Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375-5345, USA*

⁵*Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA*

⁶*Department of Physics and Department of Chemistry, University of North Texas, Denton TX*

⁷*Materials Science, Electrical Engineering, Physics and Chemistry, Duke University, Durham NC, 27708*

[†]*On leave from the Physics Department, NRCN, Israel*

***corresponding:** stefano@duke.edu

SI. VASP potentials defined in the AFLOW standard

The AFLOW standard currently relies on the set of USPP[S1, S2] and PAW[S3, S4] potentials provided with the VASP package[S5–S8]. There is often more than one potential for a given element within the available XC-functional parameterizations (LDA[S9], PW91[S10, S11], PBE[S12, S13], and rPBE[S14]), so the set used across the databases has been standardized, and is listed in Table III of the article.

The first column (‘Z’) is the atomic number of the corresponding element, the second column (‘Element’) is the IUPAC designated element name. The next two columns (labeled ‘DIR’, and ‘TITEL’) are simple identifiers assigned to a given potential by VASP; where ‘DIR’ is the name of the directory containing the files associated with the potential, and ‘TITEL’ is a text string found inside the file (e.g., at the command line, type “`grep TITEL POTCAR`”). The last column, labeled ‘md5sum’, contains the 128 bit hash of the potential files, calculated according to the procedures outlined in the RFC 1321 report[S15]. The hashes

presented here can be verified by invoking “md5sum POTCAR” at the command line.

Table S1: LDA USPP

Z	Element	DIR	TITEL	md5sum
1	H	H_soft	US H	eb925ad8f8292b2aed331bd3fe366259
3	Li	Li_pv	US Li	4c74f0df2aab6681c6744b8eaf850f28
4	Be	Be	US Be	225dec5456377fb027b46083426c573d
5	B	B	US B	b142eca3c528753dd51be9cb575d2cd3
6	C	C	US C	63c5ec5bc26ee833756991c994bf3971
7	N	N	US N	ea7c6f6f527a5fca95fd7e04c52e0a8b
8	O	O	US O	ea3fd13db24585836db99a6aeed0931
9	F	F	US F	326de96574483922f1bf3888fab704bd
10	Ne	Ne	US Ne	ebc64bf8b887fb144558f18d067bbda3
11	Na	Na_pv	NC Na	38c7cc867fdb4b3ae2074b1d672d8af7
12	Mg	Mg_pv	US Mg	82aba8531d839cebc92d493c25f9e26b
13	Al	Al	US Al	16fca2830916c80aa11e4bf5aaec1451
14	Si	Si	US Si	d99ccf54210409148cb7bc76a515a192
15	P	P	US P	d591131ae60516d08ccbc0689707f22a
16	S	S	US S	dfa02f15ca6284def141cdd5b79b6043
17	Cl	Cl	US Cl	2f00025ec1baa4a8c6d37c979919623a
18	Ar	Ar	US Ar	caa40f6e4bc306ea5f8716dd732760e9
19	K	K_pv	US K	21ff2e0252657efb7a70447c361ae6f3
20	Ca	Ca_pv	US Ca	1136d4843b98ae91d7fcfbac234cdc24
21	Sc	Sc_pv	US Sc	c5cf4ef5ccb3b6f02f82c929540cb3fd
22	Ti	Ti_pv	US Ti	20fd79c679ca800665c253449e2aaff2
23	V	V_pv	US V	1125e888772e40c79d7285ced56f17e
24	Cr	Cr	US Cr	704092fa305750c20280b1c8b1f57381
25	Mn	Mn	US Mn	ffe37780b855cb0c6bedd8abf94dd04a
26	Fe	Fe	US Fe	b61ee289bd85cad88bd9481c70bf0cce
27	Co	Co	US Co	4a9742c340a6be9ab07e4ec2c0aba71a
28	Ni	Ni	US Ni	90ea5f80a94706d35a7b00017f2eea48
29	Cu	Cu	US Cu	f3cf3dd83f64133a5b544a62ca3be702
30	Zn	Zn	US Zn	941725ce35406aa8f4ca40df9adefa74
31	Ga	Ga_d	US Ga	eb970f596dec3d1bda47a37b8c30d054
32	Ge	Ge	US Ge	99cb9eeb0ca7e512d6ea5c4105beb8bf
33	As	As	US As	b51408115da65215ae682248d4a081e2
34	Se	Se	US Se	480b2eaaf75332e764c806dd21733774
35	Br	Br	US Br	89b2c34274c20f8efa8c68328a3470ce
36	Kr	Kr	US Kr	0c33e83039365a1ddb7783b14f5c82a7
37	Rb	Rb_pv	US Rb	c3f8a7f74bb04ec0b606684a264614a3
38	Sr	Sr_pv	US Sr	3b06e61b53c19d6260ddacf80e512e24
39	Y	Y_pv	US Y	db3c69701f52c55e1fb6ed941ba40979
40	Zr	Zr_pv	US Zr	08dd343372e1aa9c267979765596f3a6
41	Nb	Nb_pv	US Nb	2f3c182389c4645a84ba4583df4d0e65

Z	Element	DIR	TITEL	md5sum
42	Mo	Mo_pv	US Mo	c3e4d496c16e4ff400d66822d3634cb7
43	Tc	Tc	US Tc	1c0878637a54be3402087aed5ea1f957
44	Ru	Ru	US Ru	ff3f1a0dc666902913217fff463f1117
45	Rh	Rh	US Rh	5d722d70c79ceb79aaf17557c0c146a0
46	Pd	Pd	US Pd	985650fa5bdfa09a60335928a55cbe8c
47	Ag	Ag	US Ag	ca44407f75bbe28536ccb54aab2903d
48	Cd	Cd	US Cd	bfc5b09a5e80617e2d16e80b14046cf
49	In	In_d	US In	476aa320d08f591e0bed065f8d5a56af
50	Sn	Sn	US Sn	6143f182786cfed76473941a501b245f
51	Sb	Sb	US Sb	b484cc8cbb354783d88aaded3ec07814
52	Te	Te	US Te	9fe9dcea0481d0e374ab8a244e321fdf
53	I	I	US I	8e7515805abe1eb98abcea7688b6e9ba
54	Xe	Xe	US Xe	1b28a4cb2512434998d4ea3007a8484a
55	Cs	Cs_pv	US Cs	dfada2d074c371c592d0e52e38fc39c2
56	Ba	Ba_pv	US Ba	dd93238fae8f388cabb9694524c7780d
72	Hf	Hf	US Hf	860d3b62205a12b49525a1d715e1ea3e
74	W	W	US W	a9b59cee55b6aae721c20a9647427926
75	Re	Re	US Re	8a68fe927b627c198536c6412e14bb44
76	Os	Os	US Os	de797260e88311fdc7adc0788fda7507
77	Ir	Ir	US Ir	becde349adf12aec562c13a70ddbe499
78	Pt	Pt	US Pt	d6a342d830c75bc5ebc63a0f3980b823
79	Au	Au	US Au	ba0e3abdc1fd77626ec6c8e68002d270
80	Hg	Hg	US Hg	3aaa62d8be49be2021e8c756c1dde17f
81	Tl	Tl_d	US Tl_d	2d5a818a22f145d6d1b17400177fa591
82	Pb	Pb	US Pb	369a0b5aebda5a1692589bd394bf4239
83	Bi	Bi	US Bi	81e3cc8bc2d01fb0da970c6235f5f379

Table S2: PW91 USPP

Z	Element	DIR	TITEL	md5sum
1	H	H_soft	US H	49b344701d738d9372888f29b8e0d105
3	Li	Li_pv	US Li	1dcfe2e618da404f09d5a54edcb6fc34
4	Be	Be	US Be	471b9403e0964e264c8d284656158821
5	B	B	US B	b666b1abe48066ba926ed1c9d8b2c0c8
6	C	C	US C	f65131829cbfb8be4b5a0aa72cd47486
7	N	N	US N	b86eeda16c14379b5cf740db3bb4995f
8	O	O	US O	70b688bdb1a9750c4e77f5fac3f702e1
9	F	F	US F	62cbfa5f1291bc1dfaf7a710c96f2952
10	Ne	Ne	US Ne	6eee0f00a3df3188935982741549abe4
11	Na	Na_pv	NC Na	bdfcc56631dac0a7bb06414f89f8e1a6
12	Mg	Mg_pv	US Mg	fc26d5d6e47791127d2b48b5d6465ed7
13	Al	Al	US Al	a16763a52da5e43988f178ae2a694d8c
14	Si	Si	US Si	e47cce7a32dc0bcf13a9a2dce87dde3f
15	P	P	US P	1cf0505abc03ffb7b1a9d96a53435ba3

Z	Element	DIR	TITEL	md5sum
16	S	S	US S	11bbaa304ba6cfdc9136d5bbf84ae3bd
17	Cl	Cl	US Cl	bb96d4f310401d743007ccf57be3a6de
18	Ar	Ar	US Ar	c27e8f5c6074c3f05bd6dfaecac84af9
19	K	K_pv	US K	981903b398cfbf64dc67dabe6fd45a29
20	Ca	Ca_pv	US Ca	e5e22945fb7173c023b43ef158bb8896
21	Sc	Sc_pv	US Sc	da13cbdce5b5b2fe9ce7f6f1a916ab0c
22	Ti	Ti_pv	US Ti	7f1010facd8517edab0414b61766674d
23	V	V_pv	US V	36e14505556e2ff991b199280175464b
24	Cr	Cr	US Cr	5b8d3fdf2095158732a4f118e62ad5ad
25	Mn	Mn	US Mn	24c6b3a1074d3ca066b7ddc4dae6541f
26	Fe	Fe	US Fe	78b9c24e72a8f7b691f63f7f3d3e82b3
27	Co	Co	US Co	29d84db0baa8b74e4b365eb41b398926
28	Ni	Ni	US Ni	cf98288758f8e0df76e7729faa5359be
29	Cu	Cu	US Cu	a6421c4d1dd4706526424b8aab7875cf
30	Zn	Zn	US Zn	84221b8c6489d29220c2e08b13d9a119
31	Ga	Ga_d	US Ga	f3bde34eb0363f885ef401a7d56c2ac3
32	Ge	Ge	US Ge	60df1a19bf0f6c7e237d393fe6b21c0c
33	As	As	US As	8d9e5cf6e9ee4da39c329da581efa904
34	Se	Se	US Se	43948e27685e956f5267da507585b401
35	Br	Br	US Br	ffed832faf9b791bbf5432532d4d5db9
36	Kr	Kr	US Kr	0c33e83039365a1ddb7783b14f5c82a7
37	Rb	Rb_pv	US Rb	66173067710aca5aa8c2e7b6db5fc6d0
38	Sr	Sr_pv	US Sr	922ed29ba450819965a499d37f2585a4
39	Y	Y_pv	US Y	ec40634146e9f436bfc044b4713a5b5a
40	Zr	Zr_pv	US Zr	bbce40b0a1f47ad690a3899f11f5cacf
41	Nb	Nb_pv	US Nb	31a5caa5656458e2b29574702d2705a2
42	Mo	Mo_pv	US Mo	427741efdc40518322fd314805e9ccd5
43	Tc	Tc	US Tc	eca73a9770d88c4d4b59dfffa91916acf
44	Ru	Ru	US Ru	a2610236af6e4ae645302ab61d240016
45	Rh	Rh	US Rh	eb4afbedfdb76bb415e5d05abc4df5ea
46	Pd	Pd	US Pd	aacd1ea5645e766bc578d70946f986fd
47	Ag	Ag	US Ag	d60cd4929088c040581084b40e4b2f94
48	Cd	Cd	US Cd	8b3cf01d5cf305e51a375218e1f63152
49	In	In_d	US In	df02b0d0b14fea4ae46bd8f9f666df64
50	Sn	Sn	US Sn	01d87027573c1dc64788aa4bc6312cae
51	Sb	Sb	US Sb	12beb615acd4ef47911327f438ba6b29
52	Te	Te	US Te	1fa179e40d92f746ef940927af58242a
53	I	I	US I	2a13ac6c3894ad9d7f128d50d0eb41a7
54	Xe	Xe	US Xe	1b28a4cb2512434998d4ea3007a8484a
55	Cs	Cs_pv	US Cs	5c6d68c09c7fd9b8b20b6a7060fc0dfc
56	Ba	Ba_pv	US Ba	b9306a9c86d23844a060e5a1d2ef1aa9
72	Hf	Hf	US Hf	142c010699d14efb38173f692cf6e8f4
73	Ta	Ta	US Ta	e6f6f719eb624ef80ed9ba4517b6059e
74	W	W	US W	98b90e789a1477f248c758e9308b28bf
75	Re	Re	US Re	25a93745d878eaad63b45a5f12db614e

Z	Element	DIR	TITEL	md5sum
76	Os	Os	US Os	129f04d303f6692a42fb802f4e2068f3
77	Ir	Ir	US Ir	5e6f57ac4035a68567e687bb3f5616a3
78	Pt	Pt	US Pt	fd17cf003dad0484f3aca9edc3b2a101
79	Au	Au	US Au	56247e2fa6201a9dc922c32d1eca5853
80	Hg	Hg	US Hg	9cb5c078d34933144ecec763122850172
81	Tl	Tl_d	US Tl_d	1391dda009434fab4a3dac58aff7c741
82	Pb	Pb	US Pb	938cdfed4297995b7e1e59bdfaeed32
83	Bi	Bi	US Bi	020b5eff92beba8759bd6031116b71b

Table S3: LDA PAW

Z	Element	DIR	TITEL	md5sum
1	H	H	PAW H 06May1998	c64ba787fed4467690fb36877e977ec0
2	He	He	PAW He 07Sep2000	3286e83bea313b7450dd8d6346f2474b
3	Li	Li_sv	PAW Li_sv 19Jan2001	2592f0ac8eb9f445a49339075daf547a
4	Be	Be_sv	PAW Be_sv 23Feb1998	77f6263acd7416ae25ad1ad4a13e10a2
5	B	B_h	PAW B_h 17Apr2000	b97195ca576223b6c21146056616c96a
6	C	C	PAW C 31May2000	29ac31aa4351a3f34d03c5d5a3003974
7	N	N	PAW N 31May2000	9e3bcba7049c1c68b251e510f4ff44b8
8	O	O	PAW O 31May2000	1e97a33e71df1c4917fa6050cd50c0c6
9	F	F	PAW F 31May2000	4fc5af0663c1aa202d6417b901f4c985
10	Ne	Ne	PAW Ne 07Sep2000	4c505754c399b52683bc0c93d5f612b0
11	Na	Na_pv	PAW Na_pv 28Sep2000	dad5cbede65d5b9dae264355a9284d9d
12	Mg	Mg_pv	PAW Mg_pv 02Mar1998	b4fb4036423c94c37ede4cebd7b4bc31
13	Al	Al	PAW Al 17Apr2000	9aeae06674ae387033981119cd1aca66
14	Si	Si	PAW Si 02Apr1999	4c7e59f235c1ffa2d680e748e7323d49
15	P	P	PAW P 21Jan2003	10819cfef53a74abcaf3a7dc99f6148b
16	S	S	PAW S 21Jan2003	9e245bb45e9785e87646b98f2ce8a0fa
17	Cl	Cl	PAW Cl 21Jan2003	c55744ba1216708ed1379cf58225b6f7
18	Ar	Ar	PAW Ar 07Sep2000	737b6200e8a07c0eed4cc9ac045f3291
19	K	K_sv	PAW K_sv 24Mar1998	28ee340cbfa8a1e3c180941174d1f5ee
20	Ca	Ca_sv	PAW Ca_sv 17Apr2000	08772677e267e5742ab515af847f7bf8
21	Sc	Sc_sv	PAW Sc_sv 07Sep2000	810b27b3c9a203f690fba0d6e45defa8
22	Ti	Ti_sv	PAW Ti_sv 07Sep2000	330371ddc4f8abc598d52de68f3c2414
23	V	V_sv	PAW V_sv 07Sep2000	446db21bf6a8039535aa8dd603466422
24	Cr	Cr_pv	PAW Cr_pv 07Sep2000	125a5e023eee2b05f14e164e6d2f23e3
25	Mn	Mn_pv	PAW Mn_pv 07Sep2000	bec18947131836968b57be507331fac6
26	Fe	Fe_pv	PAW Fe_pv 03Mar1998	6d157acdba99b6166e4e6353a40a94c
27	Co	Co	PAW Co 03Mar1998	c0ddd47ea5cf302e077fdb3f669c437
28	Ni	Ni_pv	PAW Ni_pv 19Apr2000	2f36d269dc1910fe58e98819b335fe03
29	Cu	Cu_pv	PAW Cu_pv 19Apr2000	e9e50d7d01620b388f8496ed16b20c5e
30	Zn	Zn	PAW Zn 03Mar1998	262e2b7faa6468d022a200ebe1e6d778
31	Ga	Ga_h	PAW Ga_h 21Jan2003	4b9c5eed9ef41ee625b45f7a97b6e64b
32	Ge	Ge_h	PAW Ge_h 21Jan2003	2ccdfefee986f74d8da10202f4f48a9e8

Z	Element	DIR	TITEL	md5sum
33	As	As	PAW As 03Mar1998	b80ae2d699381ffab8fdfd5978931eda
34	Se	Se	PAW Se 03Mar1998	7715381a9c3fe56d4a8987b3f653fa1b
35	Br	Br	PAW Br 03Mar1998	28a79473ffbeb64aad76c788ce31f558
36	Kr	Kr	PAW Kr 07Sep2000	b9e8a1601d319bd12a90bddf97d8fe5b
37	Rb	Rb_sv	PAW Rb_sv 10Feb1998	25bbd5117e82e405ed7194bd392d0cb1
38	Sr	Sr_sv	PAW Sr_sv 10Feb1998	b4075fc033f35af75f5db14e2d26dfd
39	Y	Y_sv	PAW Y_sv 10Feb1998	ae79bd5bc0c3952219fc1092d9a7ea88
40	Zr	Zr_sv	PAW Zr_sv 10Feb1998	efff5156d21e61bb7deae2ad191d39a1
41	Nb	Nb_sv	PAW Nb_sv 15Nov2001	96bb4057b821960864b28be8adcebfd
42	Mo	Mo_pv	PAW Mo_pv 08Jan2002	d3341b7f3223783c303368d4246d8d1f
43	Tc	Tc_pv	PAW Tc_pv 03Mar1998	93ba63ebd2b67ed0d5223d197bcd8307
44	Ru	Ru_pv	PAW Ru_pv 03Mar1998	2288b97fb7bb66b3e683940fd3f68468
45	Rh	Rh_pv	PAW Rh_pv 17Apr2000	9e334dcfcf84bc3b052eb200a075c1d0
46	Pd	Pd_pv	PAW Pd_pv 17Apr2000	e1662d7860db30ef27d97a39917510c0
47	Ag	Ag	PAW Ag 17Apr2000	ed64b160702a04a390be2cd833bfe5ab
48	Cd	Cd	PAW Cd 03Mar1998	c841d74b9ba8ec1101380f3d33dc409d
49	In	In_d	PAW In_d 11Feb1998	83e23eeaec87578503c1bf0f76b76c0f
50	Sn	Sn	PAW Sn 03Oct2001	48886f7b0a395c7a6776c1152d87e59f
51	Sb	Sb	PAW Sb 04Feb1998	e7012453f5b39f3a4dc1d82aa38e31a0
52	Te	Te	PAW Te 03Oct2001	c63d399b5887a94e071ab5ebc51ac474
53	I	I	PAW I 03Oct2001	813e041475b01902ddd9057e0096f803
54	Xe	Xe	PAW Xe 07Sep2000	f4afaa236e08c8f909f1f819778f4c4e
55	Cs	Cs_sv	PAW Cs_sv 07Sep2000	1c65ce2689c503b214f0d780b5a44e91
56	Ba	Ba_sv	PAW Ba_sv 17Apr2000	6f10884969075adfe00e752b8af4b0a7
57	La	La	PAW La 17Apr2000	112a18a4697ab2f12bbdf463f3e3e585
58	Ce	Ce	PAW Ce 28Sep2000	3bcd7760795c1bb7fccac7fb7e1f6713
72	Hf	Hf	PAW Hf 21Jan2003	a2c6186cb7d595f3e3e30235b17d7375
73	Ta	Ta_pv	PAW Ta_pv 07Sep2000	3704c06706658d369d412b5f20d07fbd
74	W	W_pv	PAW W_pv 22Jul1998	1aeee48e39ceea2ec33695b841bb3032
75	Re	Re_pv	PAW Re_pv 11Feb1998	b2422eb5ec9b7905007f5a5663f43576
76	Os	Os_pv	PAW Os_pv 10Feb1998	d62ab66828e41baf38d6d01b66fef8cd
77	Ir	Ir	PAW Ir 10Feb1998	9d79269e62a439c13853ce337e7d20c3
78	Pt	Pt	PAW Pt 17Apr2000	6f02913d6824ef5ab4014e6c48912df6
79	Au	Au	PAW Au 04Feb1998	c3f4bfdfb1e2cbe7641e47743e491adb
80	Hg	Hg	PAW Hg 04Feb1998	ffdb758a95cc239735dffbd37ff30e95
81	Tl	Tl_d	PAW Tl_d 11Feb1998	7e927afef27954355adebc00110e73c7
82	Pb	Pb_d	PAW Pb_d 30Apr1998	567fd77293c6b3213fabedc28b8a5e50
83	Bi	Bi_d	PAW Bi_d 09Feb1998	61065b58b70347893c5a90440974830b
89	Ac	Ac	PAW Ac 12Apr2000	e04fe65bdf5abd98a8498c18ad24502d
90	Th	Th_s	PAW Th_s 04May2000	f8544df429cdcf12e1b374d4cb6d231
91	Pa	Pa	PAW Pa 17Apr2000	1982b4ff040c7572783aa4aaf37f2c50
92	U	U	PAW U 17Apr2000	2e42a4a667f31bfcdfab07f2369ea452
93	Np	Np_s	PAW Np_s 04May2000	04575098e009315f819e3064f459eeb9
94	Pu	Pu_s	PAW Pu_s 04May2000	af1079053f14de3a3eed67e5fa796a42

Table S4: PW91 PAW

Z	Element	DIR	TITEL	md5sum
1	H	H	PAW_GGA H 07Jul1998	140d7a0918df4c990b60772598e7777a
2	He	He	PAW_GGA He 05Jan2001	230942b78a7aba758fa46d46df42430d
3	Li	Li_sv	PAW_GGA Li_sv 23Jan2001	ffa3b4f10c33767aa06e357f76bc1b03
4	Be	Be_sv	PAW_GGA Be_sv 23Feb1998	ead81323e7cb91242e361b2ee1883596
5	B	B_h	PAW_GGA B_h 18Jul2000	aa4fe162348dddda2a75bb20e2fcb467
6	C	C	PAW_GGA C 05Jan2001	5d9d9a5215191e6de6f5d444022eca48
7	N	N	PAW_GGA N 31May2000	c6c3f26fe10279a5a0a3cb5e6e27fbd5
8	O	O	PAW_GGA O 05Jan2001	0255483b998f590aad1e7e62c6a6216
9	F	F	PAW_GGA F 31May2000	f826add23862e81993aeb9f6f4578519
10	Ne	Ne	PAW_GGA Ne 05Jan2001	7fd5008321fbc87850280609433531df
11	Na	Na_pv	PAW_GGA Na_pv 05Jan2001	f245e8d730138b18c7caf93f34a8b14a
12	Mg	Mg_pv	PAW_GGA Mg_pv 10Feb1998	b0e3683054a3af1bcdb004403a20ec3d
13	Al	Al	PAW_GGA Al 05Jan2001	b1d947984379eb01f70e04f0b0786cc1
14	Si	Si	PAW_GGA Si 05Jan2001	fa1ca8b47f680b37e46b843a4651a032
15	P	P	PAW_GGA P 21Jan2003	51f8c161115885a5dac34b247420a44b
16	S	S	PAW_GGA S 21Jan2003	884522c45d0383c14624834330e2d638
17	Cl	Cl	PAW_GGA Cl 21Jan2003	07b6a81b71715cd88192659ca5b67446
18	Ar	Ar	PAW_GGA Ar 06Sep2000	90ed412274591809ed1a86c38d1e199c
19	K	K_sv	PAW_GGA K_sv 04May1998	868206abf76a0fc503a7eabae9a0e671
20	Ca	Ca_sv	PAW_GGA Ca_sv 04May1998	e6b809b9467f1ef0276d68a7bccc0079
21	Sc	Sc_sv	PAW_GGA Sc_sv 07Sep2000	d3fa5a5cf94262f1f318fa3d4b58abb7
22	Ti	Ti_sv	PAW_GGA Ti_sv 07Sep2000	5fe2d8774445fe6fc0e37e01bb1a6e90
23	V	V_sv	PAW_GGA V_sv 14Sep2000	52b4cc9580238169a2383464b6ff9761
24	Cr	Cr_pv	PAW_GGA Cr_pv 07Sep2000	fd46d4a02214541f586c5c278dfe5446
25	Mn	Mn_pv	PAW_GGA Mn_pv 07Sep2000	c2edf7adef8a5fbd6f981b13eb4197e9
26	Fe	Fe_pv	PAW_GGA Fe_pv 06May1998	af7f2616461457bd969597675ac6b979
27	Co	Co	PAW_GGA Co 03Mar1998	17964872269e6da2031b2c6f74ff01ac
28	Ni	Ni_pv	PAW_GGA Ni_pv 19Apr2000	1edb477085ee6c779ae372f2440ee416
29	Cu	Cu_pv	PAW_GGA Cu_pv 19Apr2000	85355af0ea6b73e2a38f987ad76414d3
30	Zn	Zn	PAW_GGA Zn 03Mar1998	a0062191fe4e00dcf6cfd024e2a3afc9
31	Ga	Ga_h	PAW_RPBE Ga_h 09Apr2002	147abcb548d98849c031596f476afb8d
32	Ge	Ge_h	PAW_RPBE Ge_h 09Apr2002	bdc0c9f007a44bd876802904c7bbe586
33	As	As	PAW_GGA As 18Jul2000	863cd990362db2801eec3eae1ffab388
34	Se	Se	PAW_GGA Se 04May1998	ae289f0158094845f991fea1e6bc3213
35	Br	Br	PAW_GGA Br 04May1998	9a8aa54e918c215c6744e86545734a0b
36	Kr	Kr	PAW_GGA Kr 07Sep2000	de3ea20f253c80645ba861128e9abb43
37	Rb	Rb_sv	PAW_GGA Rb_sv 10Feb1998	93f351b07d19603049a34f7c2119fe52
38	Sr	Sr_sv	PAW_GGA Sr_sv 10Feb1998	ed80aa48f32e3e4ef74e323b99eb68e6
39	Y	Y_sv	PAW_GGA Y_sv 10Feb1998	771600ced66e074503cdbaf6b9aa7307
40	Zr	Zr_sv	PAW_GGA Zr_sv 10Feb1998	c8b381ec47a5b1c7e2bfcbee29cdc581
41	Nb	Nb_sv	PAW_GGA Nb_sv 14Nov2001	b2b3d55a3b6e58a8cb424b89c4ce2aa1
42	Mo	Mo_pv	PAW_GGA Mo_pv 08Jan2002	d2f943e543db31280fd9a7576d4e2b0a
43	Tc	Tc_pv	PAW_GGA Tc_pv 20Feb1998	191032ad2564da987e8d595f4e39d55b

Z	Element	DIR	TITEL	md5sum
44	Ru	Ru_pv	PAW_GGA Ru_pv 10Feb1998	1b6aae0ea6dee02e54668ec33ef9d115
45	Rh	Rh_pv	PAW_GGA Rh_pv 17Apr2000	daa23016fd24638a294fa7f0c3d10e23
46	Pd	Pd_pv	PAW_GGA Pd_pv 04Mar1998	8f9d5f875d5542d128fa970f182337cd
47	Ag	Ag	PAW_GGA Ag 18Jul2000	39277c945a9786a7ddf7d5a642c969fe
48	Cd	Cd	PAW_GGA Cd 04May1998	a38ee924516dda6188855d8250d20d72
49	In	In_d	PAW_GGA In_d 04May1998	97d352df20b81868b708a5adcbf94def
50	Sn	Sn	PAW_GGA Sn 07Sep2001	c82c3f0930c9668e91889c9d570e6267
51	Sb	Sb	PAW_GGA Sb 04May1998	6d8948cd37189f4e4dd25bf2faf5be25
52	Te	Te	PAW_GGA Te 07Sep2001	91cd7274b96cf472bf9e79a6c1405d4e
53	I	I	PAW_GGA I 07Sep2001	e6bf346c007cf680c3a99d0ee59e5ff7
54	Xe	Xe	PAW_GGA Xe 07Sep2000	03a1562eb378b4d860fd567a27703dfe
55	Cs	Cs_sv	PAW_GGA Cs_sv 07Sep2000	0c18ca1ceef9d2857d92368947335ad9
56	Ba	Ba_sv	PAW_GGA Ba_sv 14Apr2000	6e953fc070f3c90dbb8ece8a4b996ba6
57	La	La	PAW_GGA La 14Apr2000	57e7cdb5a0b4016210318f2454ac21bd
58	Ce	Ce	PAW_GGA Ce 29Sep2000	93db055049ffb39a0831fae76649fc22
62	Sm	Sm_3	PAW_GGA Sm_3 11May2000	34081ab91826e45b3fbd4f9cc9399862
64	Gd	Gd_3	PAW_GGA Gd_3 10May2000	05401c5df05a5fd78f5cfa9d754005f1
65	Tb	Tb_3	PAW_GGA Tb_3 10May2000	65c0a820fda66135023edf357f7702c8
66	Dy	Dy_3	PAW_GGA Dy_3 10May2000	ca64394b868d9f2f7672d145853dcde5
67	Ho	Ho_3	PAW_GGA Ho_3 10May2000	cfdf1f1c8cd6dcc911bc74df768a507a8
68	Er	Er_3	PAW_GGA Er_3 10May2000	e48c3b9311654d5dfa43d17fe669f755
69	Tm	Tm	PAW_GGA Tm 21Aug2000	f4e0aa99eff443800adb7ddc059cb7fe
70	Yb	Yb	PAW_GGA Yb 05Sep2000	991b0c8c24181306d9150a73ddad30cd
72	Hf	Hf	PAW_GGA Hf 6May2002	3f1572eb155ff63457d12797af8834c8
73	Ta	Ta_pv	PAW_GGA Ta_pv 07Sep2000	da7bd3a2eb2d81b354149d1c59e76080
74	W	W_pv	PAW_GGA W_pv 15Jul1998	f991cc70c485b3432e5f66df766b9814
75	Re	Re_pv	PAW_GGA Re_pv 11Feb1998	16fad93aa36332c46b240dc3b8558999
76	Os	Os_pv	PAW_GGA Os_pv 10Feb1998	c73d8aaa09137dd1e4e530844ccf25c2
77	Ir	Ir	PAW_GGA Ir 04May1998	2eaff92eb3e3ba72087f9785e13f2ed7
78	Pt	Pt	PAW_GGA Pt 05Jan2001	d69e9d0cf59724336f11730eb2cd0b95
79	Au	Au	PAW_GGA Au 18Jul2000	a05903b0a24d1f0640b2622c8c676610
80	Hg	Hg	PAW_GGA Hg 04May1998	2ce3e6d38658022c51d3bdfa1244511b
81	Tl	Tl_d	PAW_GGA Tl_d 11Feb1998	2b6b043891ac43d5ab739f9623684138
82	Pb	Pb_d	PAW_GGA Pb_d 04May1998	b9da96e65065129ef12f567887580213
83	Bi	Bi_d	PAW_GGA Bi_d 10Feb1998	9fb8bff76611e718ffa9320224303393
89	Ac	Ac	PAW_GGA Ac 11Apr2000	8c84936e001650a36f2308a726c523e7
90	Th	Th_s	PAW_GGA Th_s 04May2000	a69dbeeffcef4afe95855eff44e6e297
91	Pa	Pa	PAW_GGA Pa 14Apr2000	62d018bb49199dd57f30efdc682354cc
92	U	U	PAW_GGA U 14Apr2000	6219c236d4d45ece6cbc5b677a1fcb55
93	Np	Np_s	PAW_GGA Np_s 04May2000	a5979d83571970358fba40303e0ad2a3
94	Pu	Pu_s	PAW_GGA Pu_s 04May2000	c00d31bcc05e7ce7c30165529823627e

Table S5: PBE PAW

Z	Element	DIR	TITEL	md5sum
1	H	H	PAW_PBE H 15Jun2001	0885b68e212c30cfc24e7e414f08f688
2	He	He	PAW_PBE He 05Jan2001	588ae1e19ffafb3f90f70eaf1ab0eee4
3	Li	Li_sv	PAW_PBE Li_sv 23Jan2001	3c250e93980edd21056c57109939666d
4	Be	Be_sv	PAW_PBE Be_sv 06Sep2000	3155ec5a4c068e5e462863f4fa0a4cfe
5	B	B_h	PAW_PBE B_h 07Sep2000	d9db8e5aa07a50806ed81059627ca382
6	C	C	PAW_PBE C 08Apr2002	3f40bfc49008d2f30222dd40d0a93683
7	N	N	PAW_PBE N 08Apr2002	94b576a3f411071f6852525625f70f43
8	O	O	PAW_PBE O 08Apr2002	3d1718e04592b985074657c3aa8093f0
9	F	F	PAW_PBE F 08Apr2002	7a2a358a734bd94f392dc078aa8915fa
10	Ne	Ne	PAW_PBE Ne 05Jan2001	21c1a12156171b9d49872bcf22fb3797
11	Na	Na_pv	PAW_PBE Na_pv 05Jan2001	c2bf3a84744e11107e8c18128fe55175
12	Mg	Mg_pv	PAW_PBE Mg_pv 06Sep2000	29f4a964a56871f79d918d9ed859272e
13	Al	Al	PAW_PBE Al 04Jan2001	c6620d70f1674312e1c878af213394c0
14	Si	Si	PAW_PBE Si 05Jan2001	beda35742cbd33a80c5a3dbb3b8e9dff
15	P	P	PAW_PBE P 17Jan2003	373269af03998b9ce6e4d1eb37beae32
16	S	S	PAW_PBE S 17Jan2003	7460841ca2572e68be01a43361fbc783
17	Cl	Cl	PAW_PBE Cl 17Jan2003	0400317e0e4824a73cd6da93406ea714
18	Ar	Ar	PAW_PBE Ar 07Sep2000	dd06167e63151d443b9c881a7b613693
19	K	K/_sv	PAW_PBE K_sv 06Sep2000	0ff0a8201b80271c066e28a44690c306
20	Ca	Ca_sv	PAW_PBE Ca_sv 06Sep2000	83612deb5dab8f4d5f04ad0c49b37e60
21	Sc	Sc_sv	PAW_PBE Sc_sv 07Sep2000	65fcbf4d557d3593facd06d5567ce7e1
22	Ti	Ti_sv	PAW_PBE Ti_sv 07Sep2000	9363a773551e1502ff3555eea19e9dc6
23	V	V_sv	PAW_PBE V_sv 07Sep2000	4153776e1f31baa7d48fe220244e964c
24	Cr	Cr_pv	PAW_PBE Cr_pv 07Sep2000	8813aad57bb1bc3499076346ee292337
25	Mn	Mn_pv	PAW_PBE Mn_pv 07Sep2000	f2fb52af9afe1b1c8571f5383d9ee13d
26	Fe	Fe_pv	PAW_PBE Fe_pv 06Sep2000	c6af12c1fec2e0a61c14cf46507ce36a
27	Co	Co	PAW_PBE Co 06Sep2000	fa3f50abba383404730d93936d12fd2f
28	Ni	Ni_pv	PAW_PBE Ni_pv 06Sep2000	4e3b30cbd544bb6627f6cf2b4e43eec2
29	Cu	Cu_pv	PAW_PBE Cu_pv 06Sep2000	b4736b653102363b0f0642c69492bfa4
30	Zn	Zn	PAW_PBE Zn 06Sep2000	91eb5a6b4785fe950e87899b5da3933d
31	Ga	Ga_h	PAW_PBE Ga_h 09Apr2002	00291046df22bb0f0fc1b820d319c4d3
32	Ge	Ge_h	PAW_PBE Ge_h 09Apr2002	430bc9f8543120cf365a571924b4871d
33	As	As	PAW_PBE As 06Sep2000	b56aa4c3857cd52535b010900c6ea842
34	Se	Se	PAW_PBE Se 06Sep2000	2d3bcd87e5f2e128761e12cafd90b46b
35	Br	Br	PAW_PBE Br 06Sep2000	84ffa9e5d4751de56907209cd5d85da7
36	Kr	Kr	PAW_PBE Kr 07Sep2000	ab6b338b92aa805ea896d7a440633feb
37	Rb	Rb_sv	PAW_PBE Rb_sv 06Sep2000	8c62106f12f98250f472892ee198bd9c
38	Sr	Sr_sv	PAW_PBE Sr_sv 07Sep2000	d4c83e2f1cce04c8de590ff9fee3a7b7
39	Y	Y_sv	PAW_PBE Y_sv 06Sep2000	3fd69da3d44b112b1962713a8ce3b9d9
40	Zr	Zr_sv	PAW_PBE Zr_sv 07Sep2000	4e036d1e0f59ac26bd20b213be0ce2ed
41	Nb	Nb_sv	PAW_PBE Nb_sv 17Jan2003	0f0c5358a2990a674cf95c94eb5d4be2
42	Mo	Mo_pv	PAW_PBE Mo_pv 08Apr2002	b137488ce53231ea649f1950747039d8
43	Tc	Tc_pv	PAW_PBE Tc_pv 06Sep2000	37a54b6cf59138a193b1a3f4d2b4b7dd

Z	Element	DIR	TITEL	md5sum
44	Ru	Ru_pv	PAW_PBE Ru_pv 06Sep2000	e46830387c37d5237e4bdd74f3bd3dba
45	Rh	Rh_pv	PAW_PBE Rh_pv 06Sep2000	533353e2b88e8adf9f9e2bc04d6fcc74
46	Pd	Pd_pv	PAW_PBE Pd_pv 06Sep2000	283c650e90bdd750d8cfb24b14328ad7
47	Ag	Ag	PAW_PBE Ag 06Sep2000	d8f0c080d94fd3b05649df44d48c7f4d
48	Cd	Cd	PAW_PBE Cd 06Sep2000	cceaff9f077c9bbfcf1146cadfbd2983
49	In	In_d	PAW_PBE In_d 06Sep2000	e811faa9dcd5ad520bf8997480ee425e
50	Sn	Sn	PAW_PBE Sn 08Apr2002	42a875226ea0623d4993d496d89bd704
51	Sb	Sb	PAW_PBE Sb 06Sep2000	9d89127dd693177b5ce417c7a7faade8
52	Te	Te	PAW_PBE Te 08Apr2002	36dc587b62964b6b918aa2b36e1ab1b2
53	I	I	PAW_PBE I 08Apr2002	355f755bf0fce41fad88ff61410ccdb9
54	Xe	Xe	PAW_PBE Xe 07Sep2000	733859c8f6b8883c99801774f3a20205
55	Cs	Cs_sv	PAW_PBE Cs_sv 08Apr2002	0cbfcc9c4ab7a7178c6a933f40737533
56	Ba	Ba_sv	PAW_PBE Ba_sv 06Sep2000	8565e299bf2052c5f58088383467176c
57	La	La	PAW_PBE La 06Sep2000	9647b0297cd866ab2e70c668f11cac6a
58	Ce	Ce	PAW_PBE Ce 28Sep2000	f3682f19c2bc579c9db13655fc55e3fd0
59	Pr	Pr	PAW_PBE Pr 08Apr2002	e9d2412f33dcd841b8e2bcdb45d1130f
60	Nd	Nd	PAW_PBE Nd 08Apr2002	3d8314713dcffcc0f4c7c5b4c0d8e997
61	Pm	Pm	PAW_PBE Pm 08Apr2002	3d2f5497d8de454b57cd6c297ecbb9e0
62	Sm	Sm	PAW_PBE Sm 08Apr2002	7afbc3e49b54c3d7748ff3d5ed8fde75
63	Eu	Eu	PAW_PBE Eu 08Apr2002	4e0b7f3c88ddd1230ca16540c7ea052
64	Gd	Gd	PAW_PBE Gd 08Apr2002	d7d6aedab129cf30658737c437c33c57
65	Tb	Tb_3	PAW_PBE Tb_3 06Sep2000	b05bc4baa2eb61a48ec33c52b3942b36
66	Dy	Dy_3	PAW_PBE Dy_3 06Sep2000	2cafbdd397eb4d19c0485fb96f501aeb
67	Ho	Ho_3	PAW_PBE Ho_3 06Sep2000	81adda19f97561e54ebd476ff54edb32
68	Er	Er_3	PAW_PBE Er_3 06Sep2000	efd2c87a46d71e0bde2eef44ae6b8f0
69	Tm	Tm	PAW_PBE Tm 06Sep2000	9c108f1baa6b37b61399d8786343d39f
70	Yb	Yb	PAW_PBE Yb 24Feb2003	85d6fcf3e76713c94fa8ca5c850d9613
71	Lu	Lu	PAW_PBE Lu 06Sep2000	5cfef6c87b4508f987257bea29b4877b
72	Hf	Hf	PAW_PBE Hf 20Jan2003	e36254885caf1b0fd0a0d4602f19c2d0
73	Ta	Ta_pv	PAW_PBE Ta_pv 07Sep2000	24f03b4232f2b78ebd3dd63d3149a278
74	W	W_pv	PAW_PBE W_pv 06Sep2000	b549485c40170ddc8e19c7b48f59860a
75	Re	Re_pv	PAW_PBE Re_pv 06Sep2000	1d0ee21e5719acc44001babe7e566de8
76	Os	Os_pv	PAW_PBE Os_pv 20Jan2003	74d08624f8235caef1a02b72d4a94d55
77	Ir	Ir	PAW_PBE Ir 06Sep2000	88884c01d337f00ee7193c5549b25131
78	Pt	Pt	PAW_PBE Pt 05Jan2001	079fdad3df93dbceac18c56a69852e29
79	Au	Au	PAW_PBE Au 06Sep2000	7c8b6e5d57953a616d7d99a3e5f5ff83
80	Hg	Hg	PAW_PBE Hg 06Sep2000	16228ba36308ae7834869282a95df256
81	Tl	Tl_d	PAW_PBE Tl_d 06Sep2000	8f6a3ef769f99ba50176a183fd615119
82	Pb	Pb_d	PAW_PBE Pb_d 06Sep2000	557b550dcafa40ec47cef90a84c6ae65
83	Bi	Bi_d	PAW_PBE Bi_d 06Sep2000	18f4c6d2eed662f76db6cb7ce103ca3c
89	Ac	Ac	PAW_PBE Ac 06Sep2000	2a772ba39a7528c9963370132096ae77
90	Th	Th_s	PAW_PBE Th_s 06Sep2000	509216edad7601050a1ae6fb60519dd8
91	Pa	Pa	PAW_PBE Pa 07Sep2000	584daf6e9769f685e4356a483eccd4f6
92	U	U	PAW_PBE U 06Sep2000	13e3c0dcfda26c641935253c571001e9
93	Np	Np_s	PAW_PBE Np_s 06Sep2000	af137b99591100c7827352172cf80215

Z	Element	DIR	TITEL	md5sum
94	Pu	Pu_s	PAW_PBE Pu_s 06Sep2000	500103d54c5637fc8ebb8cc8b07cfc34

- [S1] D. Vanderbilt, *Soft self-consistent pseudopotentials in a generalized eigenvalue formalism*, Phys. Rev. B **41**, 7892–7895 (1990).
- [S2] G. Kresse and J. Hafner, *Norm-Conserving and Ultrasoft Pseudopotentials for First-Row and Transition-Elements*, J. Phys.: Condens. Matt. **6**, 8245–8257 (1994).
- [S3] P. E. Blöchl, *Projector augmented-wave method*, Phys. Rev. B **50**, 17953–17979 (1994).
- [S4] G. Kresse and D. Joubert, *From ultrasoft pseudopotentials to the projector augmented-wave method*, Phys. Rev. B **59**, 1758–1775 (1999).
- [S5] G. Kresse and J. Hafner, *Ab initio molecular dynamics for liquid metals*, Phys. Rev. B **47**, 558–561 (1993).
- [S6] G. Kresse and J. Hafner, *Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium*, Phys. Rev. B **49**, 14251–14269 (1994).
- [S7] G. Kresse and J. Furthmüller, *Efficiency of ab initio total energy calculations for metals and semiconductors using a plane-wave basis set*, Comp. Mat. Sci. **6**, 15–50 (1996).
- [S8] G. Kresse and J. Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set*, Phys. Rev. B **54**, 11169–11186 (1996).
- [S9] J. P. Perdew and A. Zunger, *Self-interaction correction to density-functional approximations for many-electron systems*, Phys. Rev. B **23**, 5048–5079 (1981).
- [S10] J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais, *Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation*, Phys. Rev. B **46**, 6671–6687 (1992).
- [S11] J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais, *Erratum: Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation*, Phys. Rev. B **48**, 4978–4978 (1993).
- [S12] J. P. Perdew, K. Burke, and M. Ernzerhof, *Generalized Gradient Approximation Made Simple*, Phys. Rev. Lett. **77**, 3865–3868 (1996).
- [S13] J. P. Perdew, K. Burke, and M. Ernzerhof, *Erratum: Generalized Gradient Approximation Made Simple*, Phys. Rev. Lett. **78**, 1396–1396 (1997).
- [S14] B. Hammer, L. B. Hansen, and J. K. Nørskov, *Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals*, Phys. Rev. B **59**, 7413–7421 (1999).

[S15] R. L. Rivest, *The MD5 Message-Digest Algorithm*, RFC 1321, RFC Editor (1992).