Supplementary Material for "Deorbitalized meta-GGA Exchange-Correlation Functionals in Solids"

Daniel Mejia-Rodriguez[1,*] and S.B. Trickey[2,†]

[1] *Quantum Theory Project, Department of Physics, University of Florida, Gainesville, FL 32611*
[2] *Quantum Theory Project, Departments of Physics and of Chemistry, University of Florida, Gainesville, FL 32611*

(Dated: 5 Sep. 2018)

This supplementary material presents figures with the same data as the main text but a different representation for the interested reader. This format is the same as the one used in Reference 1. New data, from calculations of SCAN-L with the ultrasoft pseudopotentials (USPP) in VASP[2], is also included. Deviations seen between SCAN-L (PAW) and SCAN-L (USPP) are typical of the errors arising from the use of USPP[3]. Experimental values used for Figure S1 were taken from Reference 4 and those used for Figure S2 were taken from Reference 5.

* dmejiarodriguez@ufl.edu
† trickey@qtp.ufl.edu

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[3] http://www.vasp.at/vasp-workshop/slides/pseudopp2.pdf
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TABLE S1. Relative error (in %), with respect to experiment, in calculated static-lattice lattice constant, a_0, and cohesive energy, E_{coh}, for 55 solids. The experimental reference values, from Ref. 4, include zero-point effects.

Solid	a_0			E_{coh}		
	SCAN	SCAN-L	SCAN-L(USPP)	SCAN	SCAN-L	SCAN-L(USPP)
C	-0.06	0.39	0.03	0.00	-1.46	1.14
Si	0.15	0.04	0.38	0.21	-1.71	-4.66
Ge	0.43	0.41	1.71	1.29	-1.80	-4.75
Sn	0.97	1.07	2.19	3.48	2.85	2.87
SiC	0.13	0.25	-0.20	-0.46	-2.62	-1.82
BN	0.39	0.56	0.44	1.18	0.59	3.50
BP	0.00	0.11	-0.12	3.31	0.97	4.40
AlN	-0.18	-0.09	-0.80	-0.85	-1.71	-1.04
AlP	0.28	-0.04	0.07	-1.85	-3.70	-4.62
AlAs	0.39	0.18	0.66	0.52	-2.88	-2.84
GaN	-0.33	-0.16	-0.95	-3.08	-3.74	-0.17
GaP	0.13	0.11	0.68	0.28	-2.77	-1.10
GaAs	0.34	0.66	1.32	-1.50	-5.69	-2.89
InP	0.58	0.65	1.17	-8.07	-10.66	-8.11
InAs	0.78	1.03	1.60	-4.55	-8.44	-4.38
InSb	0.94	0.93	1.57	-4.63	-4.98	-5.02
LiH	0.45	-0.25	-2.09	-2.41	-2.81	0.58
LiF	0.15	0.17	0.29	-1.79	-4.26	1.04
LiCl	0.57	0.32	-0.94	-2.23	-4.46	-5.54
NaF	-0.63	-0.18	0.56	-1.76	-4.79	4.77
NaCl	-0.11	-0.49	0.31	-2.40	-4.79	-2.75
MgO	0.12	0.38	-0.36	0.77	-0.58	2.47
Li	0.41	0.78	-3.31	-6.59	-6.59	1.37
Na	-0.50	-1.69	-0.76	-7.14	-11.61	6.88
K	1.78	0.50	0.25	-13.83	-17.02	-13.49
Rb	2.39	0.88	0.84	-13.95	-19.77	-21.37
Cs	3.11	0.85	1.34	-34.57	-29.63	-23.22
Ca	-0.18	-1.44	-1.44	0.00	5.88	12.07
Ba	0.64	0.50	1.25	-22.51	2.62	-7.57
Sr	0.73	0.00	-0.87	-1.16	-1.16	3.43
Al	-0.30	-0.52	-0.38	4.08	2.62	0.43
Fe	0.07	-1.47	0.60	6.98	6.51	7.87
Co	-0.54	-0.60	0.35	6.79	-0.23	3.50
Ni	-1.37	-0.57	0.29	18.30	22.99	6.22
Sc	0.03	-0.28	0.01	0.76	-1.53	-1.49
Y	0.39	-2.53	0.54	2.96	-11.16	-12.09
Ti	-0.62	-0.58	-0.23	0.82	-1.02	6.38
Zr	0.44	0.41	0.87	-5.90	-5.26	-4.63
Hf	-0.89	0.25	-0.14	-2.48	-8.67	-1.29
V	-1.59	-1.32	-0.72	-12.15	1.68	-7.07
Nb	0.06	0.36	1.09	-16.18	-16.97	-14.79
Ta	-0.82	0.03	-0.11	6.89	-4.43	0.23
Mo	0.13	0.32	1.34	-15.45	-10.20	-20.30
W	-0.35	0.16	0.27	-6.49	-14.65	-9.81
Tc	-0.18	0.30	0.67	-6.69	-3.34	-8.78
Re	-0.51	0.62	0.53	1.24	-10.19	-3.91
Ru	-0.23	0.45	1.00	-7.98	-6.79	-11.20
Os	-0.48	0.41	0.68	3.66	4.76	-1.74
Rh	-0.21	0.61	1.33	-9.69	-2.25	-13.08
Ir	-0.44	0.65	1.21	1.29	-2.72	-2.67
Pd	0.52	0.96	1.99	5.85	3.56	-2.20
Pt	0.00	1.10	2.02	-5.79	-8.18	-12.25
Cu	-0.81	-0.70	0.59	9.97	6.27	5.12
Ag	0.47	-3.67	2.00	-6.76	-10.47	-11.70
Au	0.59	1.43	3.09	-13.32	-14.36	-21.06
MARE (%)	0.54	0.55	0.92	5.91	6.42	6.36

TABLE S2. Relative error (in %), with respect to experiment, in calculated bulk modulus, B_0, of the 44 cubic solids. The experimental values, from Ref. 5, were obtained by subtracting the zero-point phonon effect from the experimental zero-temperature values.

Solid	SCAN	SCAN-L	SCAN-L(USPP)
C	1.14	-2.66	4.68
Si	-1.58	-6.81	-10.66
Ge	-10.33	-15.99	-19.14
Sn	-6.31	-10.51	-2.57
SiC	-0.92	-2.40	-1.79
BN	-3.88	-6.63	1.24
BP	3.51	-0.54	1.07
AlN	2.96	0.10	1.84
AlP	4.58	4.58	2.52
AlAs	2.00	-1.07	-4.53
GaN	-9.17	-14.23	-18.62
GaP	-0.89	-7.59	-9.93
GaAs	-4.56	-14.47	-14.34
InP	-4.31	-9.03	-13.19
InAs	-1.37	-13.82	-5.80
InSb	-5.42	-7.38	-4.56
LiH	-9.23	-1.75	-9.98
LiF	2.10	9.04	13.37
LiCl	-9.82	10.08	-1.29
NaF	13.18	15.07	17.14
NaCl	3.99	15.94	8.70
MgO	-0.12	-3.47	-5.18
Li	28.24	31.30	-15.27
Na	1.27	12.66	34.18
K	-10.53	31.58	-13.16
Rb	-25.00	-8.33	36.11
Cs	-17.39	4.35	-4.35
Ca	10.69	25.79	18.24
Ba	-21.70	-6.60	-11.32
Sr	-5.00	1.67	1.67
Al	0.52	17.38	2.85
Ni	20.88	13.87	5.19
V	18.09	17.91	18.52
Nb	2.25	4.16	1.96
Ta	2.71	-0.84	1.38
Mo	-0.33	-2.14	-10.39
W	0.18	-5.34	-4.15
Rh	5.92	-8.19	-3.83
Ir	12.42	-1.44	-6.52
Pd	2.88	1.50	-5.88
Pt	2.21	-12.57	-18.84
Cu	13.86	12.34	10.12
Ag	4.73	-5.20	-4.82
Au	-7.03	-15.60	-31.87
MARE (%)	7.2	9.4	9.8

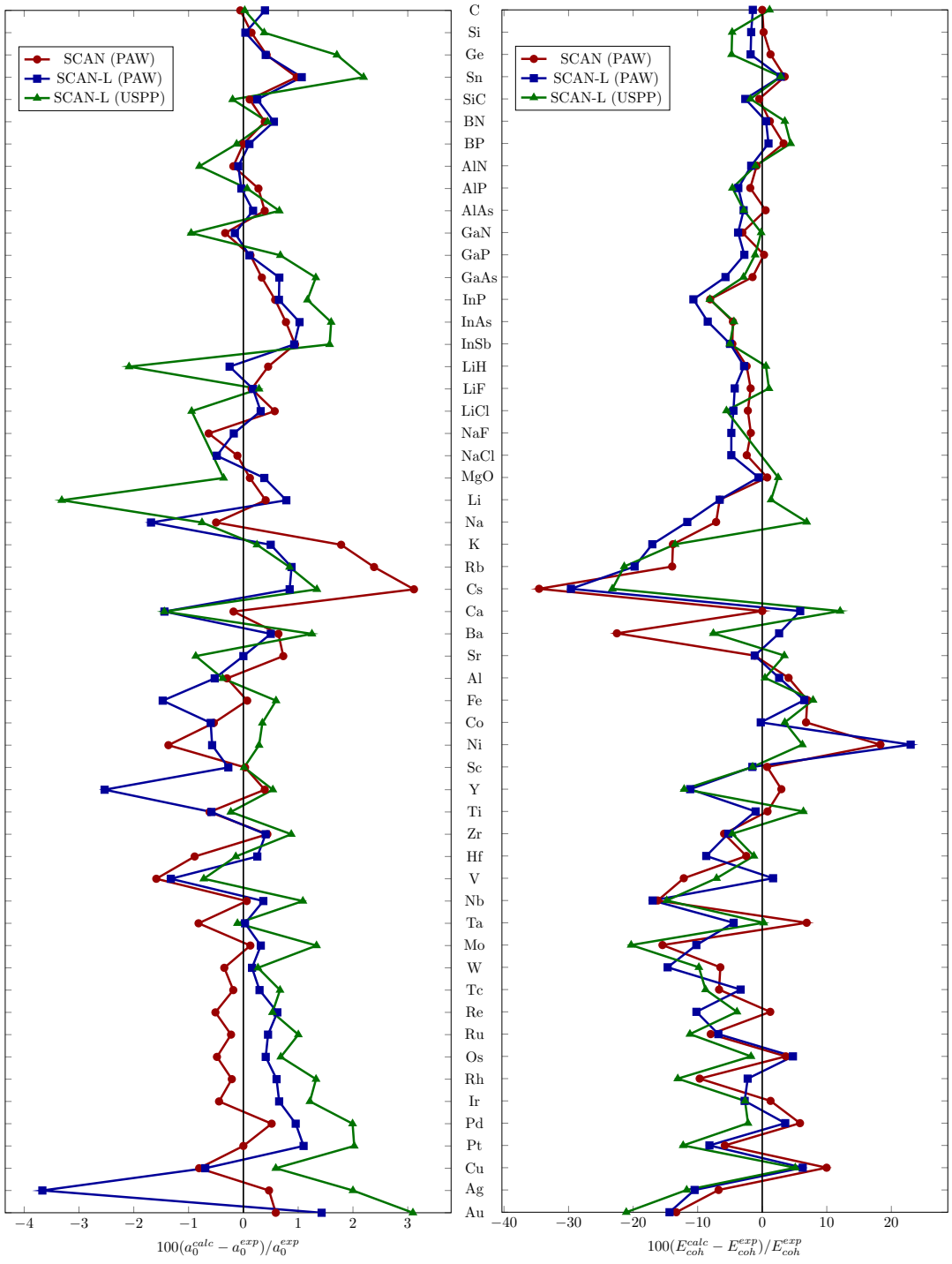

FIG. S1. Relative error (in %) with respect to experiment in the calculated lattice constant (left panel) and cohesive energy (right panel) for the 55 solids presented in the main text.

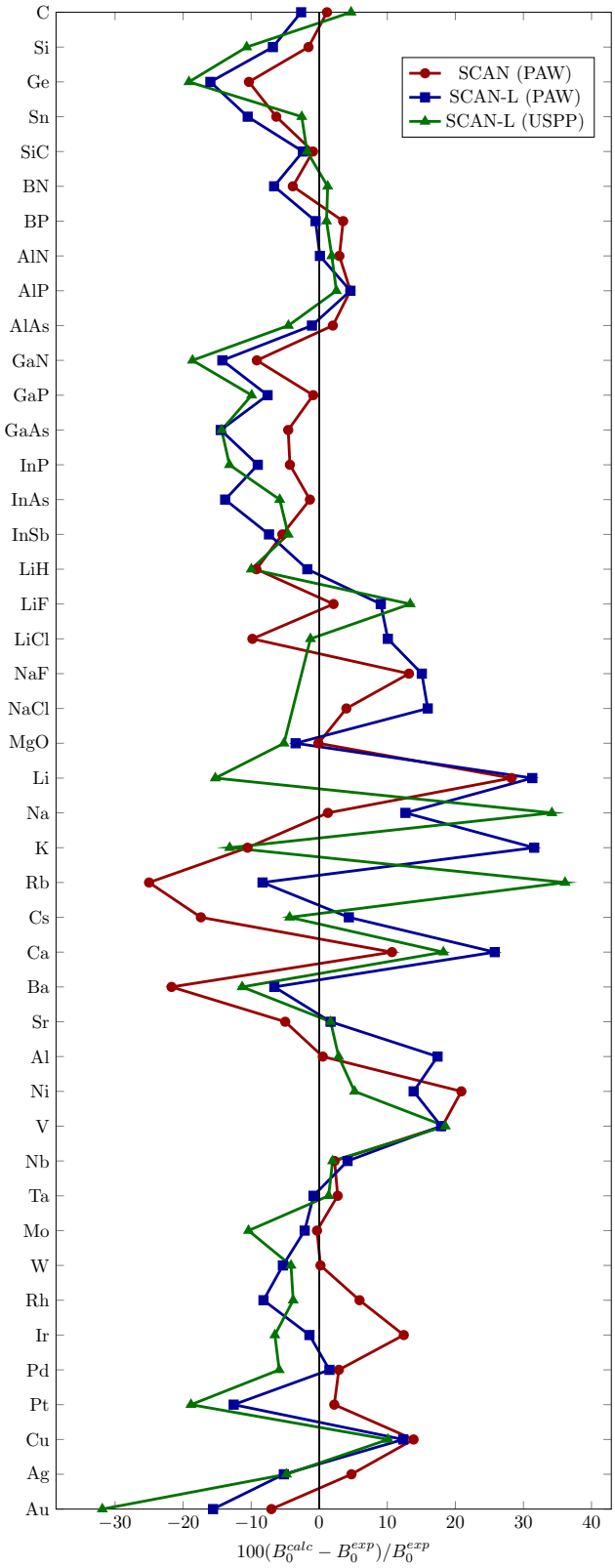

FIG. S2. Relative error (in %) with respect to experiment in the calculated Bulk modulus for the 44 solids presented in the main text.