Supplementary information to "Large-scale benchmark of exchange-correlation functionals for the determination of electronic band gaps of solids"

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Figure S1: Spin-orbit coupling shift, $\Delta_{\text{SOC}} = E_g^{\text{SOC}} - E_g^{\text{no SOC}}$ as a function of experimental gap, for LDA, PBE and HLE16. The corresponding histograms are also indicated for each distribution. No major qualitative differences distinguish the three functionals, but there are quantitative differences between HLE16 and LDA/PBE if we compare the mean value (LDA: -0.08 eV; PBE: -0.09 eV; HLE16: -0.14 eV) and the standard deviation of the distributions (LDA: 0.13 eV; PBE: 0.13 eV; HLE16: 0.22 eV). In specific cases the correction can double from LDA/PBE to HLE16, as mentioned in the main text.



Figure S2: Dispersion of band gaps calculated with PBE vs. PBEsol, displayed in logarithmic scale. In orange, the linear fit f(x) = a * x + b to this data, with a = 0.9877 and b = -0.05155. The line y = x is added as a guide to the eye.

Figure S3: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: LDA calculations. Lower panel: PBE calculations. Gray cases indicate that there are no materials containing the corresponding element.

	IA																	VIIIA
1	1 H (42)	IIA	_	L	_D/	4							IIIA	IVA	VA	VIA	VIIA	² He
2	3 Li (44)	4 Be (40)		0	39	78 11	17 14	3					5 B (41)	6 C (41)	7 N (54)	8 0 (44)	9 F (40)	10 Ne (47)
3	11 Na (36)	12 Mg (54)	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	13 Al (43)	14 Si (45)	15 P (46)	16 S (48)	17 Cl (33)	18 Ar (42)
4	19 K (42)	20 Ca (48)	21 Sc (66)	22 Ti (35)	²³ V (31)	24 Cr (19)	²⁵ Mn	26 Fe (28)	27 Co (57)	28 Ni (114)	29 Cu (67)	30 Zn (59)	31 Ga (58)	32 Ge (69)	33 As (62)	34 Se (58)	35 Br (35)	36 Kr (42)
5	37 Rb (39)	³⁸ Sr (41)	39 Y (43)	40 Zr (45)	41 Nb (21)	42 Mo (24)	⁴³ Tc	44 Ru (62)	⁴⁵ Rh	46 Pd (87)	47 Ag (64)	48 Cd (53)	49 In (62)	50 Sn (62)	51 Sb (55)	52 Te (51)	53 (36)	54 Xe (38)
6	55 Cs (35)	56 Ba (48)	57-71 La-Lu	72 Hf (48)	73 Ta (37)	74 W (28)	75 Re (14)	76 Os (52)	⁷⁷ lr	78 Pt (87)	79 Au (56)	80 Hg (52)	81 Tl (53)	82 Pb (41)	83 Bi (27)	⁸⁴ Po	At	Rn
				57 La	⁵⁸ Ce	⁵⁹ Pr	⁶⁰ Nd	61 Pm	⁶² Sm	Eu	Gd ⁶⁴ Gd	65 Tb	66 Dy	67 Ho	⁶⁸ Er	⁶⁹ Tm	⁷⁰ Yb	⁷¹ Lu
				89 Ac	90 Th (57)	91 Pa	⁹² U	⁹³ Np	⁹⁴ Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	¹⁰⁰ Fm	¹⁰¹ Md	102 No	103 Lr
	IA																	VIIIA
1	IA 1 H (36)	IIA		F	PBE	Ξ							IIIA	IVA	VA	VIA	VIIA	VIIIA ² He
1	IA 1 H (36) 3 Li (39)	11A 4 Be (38)		F	PBE		17 14	3					111A 5 B (39)	IVА 6 С (39)	VA 7 N (52)	VIA 8 0 (41)	VIIA 9 F (37)	VIIIA ² He ¹⁰ Ne (46)
1 2 3	IA 1 H (36) 3 Li (39) 11 Na (37)	11A 4 Be (38) 12 Mg (50)	IIIB	F 0 IVB	р ВЕ 39 2 VB	78 1 [^] VIB	17 14 VIIB	3 VIIIB	VIIIB	VIIIB	IB	IIB	111A 5 B (39) 13 AL (39)	IVA ⁶ <u>C</u> (39) ¹⁴ <u>Si</u> (40)	VA 7 N (52) 15 P (41)	VIA 8 0 (41) 16 5 (43)	VIIA 9 F (37) 17 CL (28)	VIIIA ² He ¹⁰ Ne (46) ¹⁸ Ar (38)
1 2 3 4	IA 1 H (36) 3 Li (39) 11 Na (37) 19 K (36)	A 4 Be (38) 12 Mg (50) 20 Ca (46)	IIIB 21 Sc (63)	0 IVB 22 Ti (32)	PBE 39 : VB	78 11 VIB 24 Cr (22)	VIIB 25 Mn	3 VIIIB ²⁶ Fe (18)	VIIIB 27 Co (47)	VIIIB 28 Ni (124)	1B 29 Cu (63)	11B 30 Zn (52)	111A 5 B (39) 13 Al (39) 31 Ga (49)	IVA ⁶ <u>C</u> (39) ¹⁴ <u>Si</u> (40) ³² <u>Ge</u> (64)	VA 7 N (52) 15 P (41) 33 As (55)	VIA ⁸ 0 (41) ¹⁶ S (43) ³⁴ Se (52)	VIIA 9 F (37) 17 Cl (28) 35 Br (30)	VIIIA ² He ¹⁰ Ne ⁽⁴⁶⁾ ¹⁸ Ar ⁽³⁸⁾ ³⁶ Kr ⁽³⁷⁾
1 2 3 4 5	IA 1 H (36) 3 Li (39) 11 Na (37) 19 K (36) 37 Rb (35)	11A 4 Be (38) 12 Mg (50) 20 Ca (46) 38 Sr (39)	111B 21 Sc (63) 39 Y (55)	0 IVB ²² Ti (32) ⁴⁰ Zr (45)	39 39 30 50 50 50 50 50 50 50 50 50 50 50 50 50	78 1 VIB 24 Cr (22) 42 Mo (21)	VIIB 25 Mn 43 Tc	3 VIIIB 26 Fe (18) 44 Ru (54)	VIIIB 27 Co (47) 45 Rh	VIIIB 28 Ni (124) 46 Pd (81)	1B 29 Cu (63) 47 Ag (57)	11B 30 Zn (52) 48 Cd (45)	111A 5 8 (39) 13 AL (39) 31 Ga (49) 10 (55)	IVA ⁶ C (39) ¹⁴ Si (40) ³² Ge (64) ⁵⁰ Sn (58)	VA 7 N (52) 15 P (41) 33 As (55) 51 Sb (52)	VIA ⁸ 0 (41) ¹⁶ 5 (43) ³⁴ 52 Te (48)	VIIA 9 F (37) 17 CL (28) 35 Br (30) 53 I (33)	VIIIA ² He ¹⁰ Ne (46) ¹⁸ Ar (38) ³⁶ Kr (37) ⁵⁴ Xe (33)
1 2 3 4 5 6	IA 1 H (36) 3 Li (37) 19 K (36) 37 Rb (35) 55 Cs (30)	IIA 4 Be (39) 20 Ca (46) 38 Sr 56 Ba (43)	IIIB ²¹ Sc (63) ³⁹ Y (57-71 La-Lu	0 IVB 22 Ti (32) 40 Zr (45) 72 Hf (42)	239 7 VB 23 VB 23 V (27) 41 Nb (19) 73 Ta (33)	78 11 ∨IB ²⁴ Cr (22) ⁴² Mo (21) ⁷⁴ W (24)	VIIB 25 Mn 43 Tc 75 Re (11)	3 VIIIB 26 Fe (18) 44 Ru (54) 76 Os (56)	VIIIB 27 Co (47) 45 Rh 777 Ir	VIIIB 28 Ni (124) 46 Pd (81) 78 Pt (130)	1B 29 Cu (63) 47 Ag (57) 79 Au (52)	30 Zn (52) 48 Cd 80 Hg (44)	111A 5 B (39) 13 AL (39) 31 Ca (49) 49 In (55) 81 TL (47)	IVA ⁶ (39) ¹⁴ Si (40) ³² Ge (64) ⁵⁰ Sn (58) ⁸² Pb (42)	VA 7 N (52) 15 P (41) 33 As (55) 51 Sb (52) 83 Bi (23)	VIA ⁸ 0 (41) ¹⁶ S (43) ³⁴ Se (52) ⁵² Te (48) ⁸⁴ Po	VIIA 9 F (37) 17 CL (28) 35 Br (30) 53 I (33) 85 At	VIIIA ² He ¹⁰ Ne (46) ¹⁸ Ar (37) ³⁶ Kr (37) ⁵⁴ Xe (33) ⁸⁶ Rn
1 2 3 4 5 6	IA 1 (36) 3 Li (37) 19 K (36) 37 Rb (35) 55 Cs (30)	11A 4 Be (38) 12 Mg (50) 20 Ca (46) 38 Sr (39) 56 Ba (43)	IIIB 21 Sc (63) 39 Y (55) 57-71 La-Lu	0 IVB 22 Ti (32) 40 Zr (45) 72 Hf (42) 72 Hf (43)	B B B B B B B B B B B B B B B B B B B	78 1 VIB 24 Cr (22) 42 Mo (21) 74 W (24) 59 Pr	VIIB 25 Mn 43 Tc 75 Re (11) 60 Nd	3 VIIIB 26 Fe (18) 44 Ru (54) 76 Os (56)	VIIIB 27 Co (47) 45 Rh 77 Ir 62 Sm	VIIIB 28 Ni (124) 46 Pd (81) 78 Pt (130) 63 Eu	1B 29 Cu (63) 47 Ag (57) 79 Au (52) 64 Gd	11B 30 Zn (52) 48 Cd (45) 80 Hg (44) 65 Tb	IIIA 5 B (39) 13 AI (39) 31 Ga (49) I I I I I I I I	IVA ⁶ (39) ¹⁴ ⁵⁰ ³² ⁶ (64) ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁰ ⁶⁰ ⁶¹	VA 7 N (52) 15 P (41) 33 As (55) 51 Sb (52) 83 Bi (23) 83 Bi (23)	VIA ⁸ 0 (41) ¹⁶ S (52) ⁵² Te (48) ⁸⁴ Po ⁶⁹ Tm	VIIA 9 F (37) 17 CL (28) 35 Br (30) 53 I (33) 85 At 70 Yb	VIIIA ² He ¹⁰ Ne ⁽⁴⁶⁾ ¹⁸ Ar ⁽³⁸⁾ ³⁶ Kr ⁵⁴ Xe ⁽³³⁾ ⁸⁶ Rn ⁷¹ Lu

Figure S4: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: HLE16 calculations without spin-orbit coupling. Lower panel: HLE16 calculations including spin-orbit coupling. Gray cases indicate that there are no materials containing the corresponding element.

	IA	_																VIIIA
1	1 H (17)	IIA		H	LE1	6							IIIA	IVA	VA	VIA	VIIA	² He
2	3 Li (23)	4 Be (20)		0	39 7	78 11	17 14	3					5 B (21)	6 C (22)	7 N (22)	8 0 (36)	9 F (18)	10 Ne (30)
3	11 Na (33)	12 Mg (16)	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	13 Al (12)	14 Si (16)	15 P (19)	16 S (25)	17 Cl (17)	18 Ar (17)
4	19 K (23)	20 Ca (32)	21 Sc (39)	22 Ti (36)	23 V (28)	24 Cr (13)	²⁵ Mn	26 Fe (31)	27 Co (72)	28 Ni (89)	29 Cu (33)	30 Zn (26)	31 Ga (21)	32 Ge (34)	33 As (34)	34 Se (46)	35 Br (17)	36 Kr (13)
5	37 Rb (20)	38 Sr (24)	39 Y (36)	40 Zr (39)	41 Nb (19)	42 Mo (13)	⁴³ Tc	44 Ru (13)	⁴⁵ Rh	46 Pd (123)	47 Ag (26)	48 Cd (23)	49 In (31)	50 Sn (36)	51 Sb (30)	52 Te (46)	53 (25)	54 Xe (4)
6	55 Cs (26)	56 Ba (20)	57-71 La-Lu	72 Hf (29)	73 Ta (33)	74 W (12)	75 Re (11)	76 Os (39)	77 Ir	78 Pt (89)	79 Au (33)	80 Hg (25)	81 Tl (24)	82 Pb (131)	83 Bi (41)	⁸⁴ Po	⁸⁵ At	Rn
				57 La	⁵⁸ Ce	⁵⁹ Pr	⁶⁰ Nd	61 Pm	⁶² Sm	Eu	G4 Gd	65 Tb	66 Dy	67 Ho	⁶⁸ Er	⁶⁹ Tm	70 Yb	⁷¹ Lu
				⁸⁹ Ac	90 Th (47)	91 Pa	⁹² U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	¹⁰⁰ Fm	¹⁰¹ Md	102 No	103 Lr
										11	11	11			11			
	IA	_																VIIIA
1	IA 1 H (17)	IIA	HL	.E1	6 (S 0) (C)						IIIA	IVA	VA	VIA	VIIA	VIIIA ² He
1	IA 1 H (17) 3 Li (25)	11A 4 Be (17)	HL	.E1	6 (SO 78 1′	C)	3					111A 5 B (21)	1VA 6 (22)	VA 7 N (26)	VIA 8 0 (39)	VIIA 9 F (21)	VIIIA ² He ¹⁰ Ne (31)
1 2 3	IA 1 H (17) 3 Li (25) 11 Na (35)	11A 4 Be (17) 12 Mg (21)	HIL	.E1 0	6 (39 7	SO 78 1′ VIB	0 C) 17 14 VIIB	3 VIIIB	VIIIB	VIIIB	IB	IIB	111A 5 B (21) 13 Al (13)	IVA ⁶ <u>C</u> (22) ¹⁴ <u>Si</u> (15)	VA 7 N (26) 15 P (21)	VIA 8 (39) 16 S (24)	VIIA 9 F (21) 17 CL (14)	VIIIA ² He ¹⁰ ¹⁰ ¹⁰ ¹⁰ ¹³ ¹⁸ Ar ⁽¹⁷⁾
1 2 3 4	IA 1 H (17) 3 Li (25) 11 Na (35) 19 K (20)	11A 4 Be (17) 12 Mg (21) 20 Ca (33)	HIL IIIB ²¹ Sc (38)	E1 0 IVB 22 Ti (36)	6 (39 7 VB	SO 78 11 VIB 24 Cr (11)	17 14 VIIB ²⁵ Mn	3 VIIIB ²⁶ Fe (43)	VIIIB 27 Co (75)	VIIIB 28 Ni (70)	1B 29 Cu (37)	11B 30 Zn (26)	111A 5 8 (21) 13 Al (13) 31 Ca (22)	IVA ⁶ (22) ¹⁴ Si (15) ³² Ge (35)	VA 7 N (26) 15 P (21) 33 As (40)	VIA ⁸ 0 (39) ¹⁶ 5 (24) ³⁴ 5 (38)	VIIA 9 F (21) 17 Cl (14) 35 Br (17)	VIIIA ² He ¹⁰ Ne (31) ¹⁸ Ar (17) ³⁶ Kr (15)
1 2 3 4 5	IA 1 H (17) 3 Li (25) 11 Na (35) 19 K (20) 37 Rb (20)	A 4 Be (17) 12 Mg (21) 20 Ca (33) 38 Sr (26)	HLL IIIB ²¹ Sc (38) ³⁹ Y (25)	E1 0 IVB ²² Ti (36) ⁴⁰ Zr (40)	6 (39 7 VB ²³ V (29) ⁴¹ Nb (20)	SO 78 1 VIB 24 Cr (11) 42 Mo (13)	C) 17 14 VIIB ²⁵ Mn ⁴³ Tc	3 VIIIB 26 Fe (43) (14)	VIIIB 27 Co (75) 45 Rh	VIIIB 28 Ni (70) 46 Pd (120)	1B 29 Cu (37) 47 Ag (26)	11B 30 Zn (26) 48 Cd (22)	111A 5 8 (21) 13 AL (13) 31 (23) 49 1 (28)	IVA ⁶ C (22) ¹⁴ Si (15) ³² Ge (35) ⁵⁰ Sn (40)	VA 7 N (26) 15 P (21) 33 As (40) 51 Sb (31)	VIA ⁸ ⁽³⁹⁾ ¹⁶ ⁵² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷² ⁷³ ⁷³ ⁷³ ⁷⁴ ⁷⁵ ⁷⁴ ⁷⁵	VIIA 9 F (21) 17 CL (14) 35 Br (17) 53 I (20)	VIIIA ² He ¹⁰ Ne (31) ¹⁸ Ar (17) ³⁶ Kr (15) ⁵⁴ Xe (10)
1 2 3 4 5 6	IA I H (72) I I I I I I I I K (25) I I I K (25) I I I K (25) I I I K (25) I I I I I I I I I I I I I	11A 4 Be (17) 12 Mg (21) 20 Ca (33) 38 Sr (26) 56 Ba (21)	IIIB ²¹ Sc (38) ³⁹ Y (25) ⁵⁷⁻⁷¹ La-Lu	E1 0 1VB 22 Ti (36) 40 Zr (40 Zr (40) 72 Hf (32)	6 (39 7 VB ²³ V (29) ⁴¹ Nb (20) ⁷³ Ta (37)	SO 78 11 VIB 24 Cr (11) 42 Mo (13) 74 W (11)	C) 17 14 VIIB ²⁵ Mn ⁴³ Tc ⁷⁵ Re (25)	3 26 Fe (43) 44 Ru (14) 76 Os (51)	VIIIB 27 Co (75) 45 Rh 77 Ir	VIIIB 28 Ni (70) 46 Pd (120) 78 Pt (73)	1B 29 Cu (37) 47 Ag (26) 79 Au (36)	11B 30 Zn (26) 48 Cd (22) 80 Hg (26)	111A 5 B (21) 13 AL (13) 13 AL (13) 31 Caa (22) 49 In (28) 81 TL (18)	IVA ⁶ (22) 14 Si (15) 32 Ge (35) 50 Sn (40) 82 Pb (57)	VA 7 N (20) 15 P (21) 33 As (40) 51 Sb (31) 83 Bi (22)	VIA ⁸ 0 (39) ¹⁶ S (24) ³⁴ Se (38) ⁵² Te (26) ⁸⁴ Po	VIIA 9 F (21) 17 CL (14) 35 Br (17) 53 I (20) 85 At	VIIIA ² He ¹⁰ Ne (31) ¹⁸ Ar (17) ³⁶ Kr (15) ⁵⁴ Xe (10) ⁸⁶ Rn
1 2 3 4 5 6	IA 1 H (17) 3 Li (25) 11 Na (35) 19 K (20) 37 Rb (20) 55 Cs (25)	11A 4 Be (17) 12 Mg (21) 20 Ca (33) 38 Sr (26) 56 Ba (21)	HIL 111B 21 Sc (38) 39 Y (25) 57-71 La-Lu	E1 0 IVB 22 Ti (36) 40 Zr (40) 72 Hf (32) 57 La (20)	6 (39 7 VB ²³ V (29) ⁴¹ Nb (20) 73 Ta (37) 58 Ce	SO 78 1 ⁻ VIB ²⁴ Cr (11) ⁴² Mo (13) 7 ⁴ W (11) ⁵⁹ Pr	C) 17 14 VIIB ²⁵ Mn ⁴³ Tc ⁷⁵ Re (25) ⁶⁰ Nd	3 26 Fe (43) 44 Ru (14) 76 Os (51) 61 Pm	VIIIB 27 Co (75) 45 Rh 77 Ir 62 Sm	VIIIB 28 Ni (70) 46 Pd (120) 78 Pt (73) 63 Eu	1B 29 Cu (37) 47 Ag (26) 79 Au (36) 64 Gd	11B 30 Zn (26) 48 Cd (22) 80 Hg (26) 65 Tb	111A 5 B (21) 13 AL (13) 31 Ca (22) 49 In (28) 81 TL (18) 66 Dy	IVA ⁶ C (22) ¹⁴ Si (15) ³² Ge (35) ⁵⁰ Sn (40) ⁸² Pb (57) ⁶⁷ Ho	VA 7 N (26) 15 P (21) 33 As (40) 51 Sb (31) 83 Bi (22)	VIA ⁸ 0 (39) ¹⁶ 5 (24) ³⁴ 5 7 6 7 7 7 7 7 7 7 7	VIIA 9 F (21) 17 Cl (14) 35 Br (17) 53 I (20) 85 At 70 Yb (100)	VIIIA ² He ¹⁰ Ne (31) ¹⁸ Ar (17) ³⁶ Kr (15) ⁵⁴ Xe (10) ⁸⁶ Rn ⁷¹ Lu

Figure S5: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: MBJ calculations. Lower panel: HSE06 calculations. Gray cases indicate that there are no materials containing the corresponding element.

	IA																	VIIIA
1	1 H (5)	IIA	_	i	nΒ	J							IIIA	IVA	VA	VIA	VIIA	² He
2	3 Li (16)	4 Be (18)		0	39	78 1´	17 14	3					5 B (24)	6 C (17)	7 N (10)	8 0 (26)	9 F (18)	10 Ne (12)
3	11 Na (25)	12 Mg (10)	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	13 Al (14)	14 Si (19)	15 P (21)	16 S (25)	17 Cl (16)	18 Ar (11)
4	19 K (23)	20 Ca (26)	21 Sc (47)	22 Ti (12)	23 V (9)	24 Cr (34)	²⁵ Mn	26 Fe (91)	27 Co (66)	28 Ni (152)	29 Cu (41)	30 Zn (16)	31 Ga (17)	32 Ge (27)	33 As (24)	34 Se (41)	35 Br (18)	³⁶ Kr (8)
5	37 Rb (19)	³⁸ Sr ₍₂₄₎	39 Y (77)	40 Zr (42)	41 Nb (14)	42 Mo (15)	⁴³ Tc	44 Ru (18)	⁴⁵ Rh	46 Pd (132)	47 Ag (30)	48 Cd (22)	49 In (37)	50 Sn (32)	51 Sb (42)	52 Te (41)	53 (25)	54 Xe (12)
6	55 Cs (24)	56 Ba (21)	57-71 La-Lu	72 Hf (7)	73 Ta (9)	74 W (8)	75 Re (3)	76 Os (68)	77 Ir	78 Pt (189)	79 Au (39)	80 Hg (15)	81 Tl (24)	82 Pb (84)	83 Bi (40)	⁸⁴ Po	⁸⁵ At	Rn
				57 La	58 Ce	⁵⁹ Pr	⁶⁰ Nd	61 Pm	⁶² Sm	Eu	G4 Gd	65 Tb	66 Dy	67 Ho	Er	⁶⁹ Tm	⁷⁰ Yb	⁷¹ Lu
				⁸⁹ Ac	90 Th	91 Pa	⁹² U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	⁹⁸ Cf	99 Es	¹⁰⁰ Fm	¹⁰¹ Md	102 No	¹⁰³ Lr
					1 N 19													
	IA																	VIIIA
1	IA 1 H (14)	IIA		H	SE(06							IIIA	IVA	VA	VIA	VIIA	VIIIA ² He
1	IA I H (14) 3 Li (21)	4 Be (19)	1	H 0	SE(06 ⁷⁸ 1′	17 14	3					111A 5 (18)	IVА 6 С (18)	VA 7 N (11)	VIA 8 0 (27)	VIIA 9 F (20)	VIIIA ² He ¹⁰ Ne (33)
1 2 3	IA 1 H (14) 3 Li (21) 11 Na (32)	11A 4 Be (19) 12 Mg (16)	IIIB	H 0 IVB	SE(39	06 78 1 VIB	17 14 VIIB	3 VIIIB	VIIIB	VIIIB	IB	IIB	111A 5 B (18) 13 Al (9)	IVA ⁶ <u>C</u> (18) ¹⁴ <u>Si</u> (29)	VA 7 N (11) 15 P (30)	VIA 8 0 (27) 16 S (23)	VIIA 9 F (20) 17 CL (18)	VIIIA ² He ¹⁰ Ne ⁽³³⁾ ¹⁸ Ar ⁽²⁷⁾
1 2 3 4	IA 1 H (14) 3 Li (21) 11 Na (32) 19 K (20)	IIA 4 Be (19) 12 Mg (16) 20 Ca (23)	111B 21 5c (74)	0 IVB 22 Ti (15)	SE(39 7 VB	D6 78 11 VIB 24 Cr (118)	VIIB 25 Mn	3 VIIIB 26 Fe (263)	VIIIB 27 Co (100)	VIIIB 28 Ni (227)	1B 29 Cu (23)	11B 30 Zn (15)	111A 5 8 (18) 13 Al (9) 31 Ca (14)	IVA 6 C (18) 14 Si (29) 32 Ge (19)	VA 7 N (11) 15 P (30) 33 As (20)	VIA 8 0(27) 16 5(23) 34 5e(37)	VIIA 9 F (20) 17 CL (18) 35 Br (20)	VIIIA ² He ¹⁰ Ne (33) ¹⁸ Ar (27) ³⁶ Kr (25)
1 2 3 4 5	IA 1 H (14) 1 1 1 Na (32) 19 K (20) 37 Rb (27)	11A Be (19) 12 Mg (16) 20 Ca (23) 38 Sr (23)	111B 21 Sc (74) 39 Y (120)	0 IVB ²² Ti (15) ⁴⁰ Zr (38)	SE 39 2 VB 23 V (32) 41 Nb (20)	D6 78 11 VIB ²⁴ Cr (118) ⁴² Mo (22)	17 14 VIIB ²⁵ Mn ⁴³ Tc	3 VIIIB 26 Fe (263) 44 Ru (49)	VIIIB 27 Co (100) 45 Rh	VIIIB 28 Ni (227) 46 Pd (170)	1B 29 Cu (23) 47 Ag (38)	11B 30 Zn (15) 48 Cd (18)	111A 5 B (18) 13 Al (9) 31 Gaa (14) 49 In (35)	IVA ⁶ C (18) ¹⁴ Si (29) ³² Ge (19) ⁵⁰ Sn (28)	VA 7 N (11) 15 P (30) 33 As (20) 51 Sb (52)	VIA 8 0 (27) 16 5 (23) 34 52 Te (42)	VIIA 9 F (20) 17 CL (18) 35 Br (20) 53 I (28)	VIIIA ² He ¹⁰ Ne ⁽³³⁾ ¹⁸ Ar ⁽²⁷⁾ ³⁶ Kr ⁽²⁵⁾ ⁵⁴ Xe ⁽²¹⁾
1 2 3 4 5 6	IA I H (14) I H (21) I1 Na (32) I1 K (20) I1 K (20) I1 S Cs (21)	IIA 4 Be (19) 12 Mg (16) 20 Caa (23) 38 Sr 56 Ba (17)	111B 21 Sc (74) 39 Y (120) 57-71 La-Lu	0 IVB 22 Ti (15) 40 Zr (38) 72 Hf (4)	39 2 VB 23 V (32) 41 Nb (20) 73 Ta (18)	D6 78 11 VIB 24 Cr (118) 42 Mo (22) 74 W (11)	VIIB 25 Mn 43 Tc 75 Re (36)	3 VIIIB 26 Fe (263) 44 Ru (49) 76 Os (149)	VIIIB 27 Co (100) 45 Rh 77 Ir	VIIIB 28 Ni (227) 46 Pd (170) 78 Pt (242)	1B 29 Cu (23) 47 Ag (38) 79 Au (28)	11B 30 Zn (15) 48 Cd (18) B0 Hg (15)	111A 5 B (18) 13 AL (9) 31 Caa (14) 49 In (35) 81 TL (23)	IVA ⁶ C (18) ¹⁴ Si (29) ³² Ce (19) ⁵⁰ Sn (28) ⁸² Pb (66)	VA 7 N (11) 15 P (30) 33 As (20) 51 Sb (52) 83 Bi (49)	VIA ⁸ 0 (27) ¹⁶ S (23) ³⁴ Se (37) ⁵² Te (42) ⁸⁴ Po	VIIA 9 F (20) 17 CL (18) 35 Br (20) 53 L (28) 85 At	VIIIA ² He ¹⁰ Ne ⁽³³⁾ ¹⁸ Ar ⁽²⁷⁾ ³⁶ Kr ⁽²⁵⁾ ⁵⁴ Xe ⁽²¹⁾ ⁸⁶ Rn
1 2 3 4 5 6	IA I H (14) I H (21) II Na (32) II K (20) II S Cs (21)	IIA Be (19) I2 Mg (16) 20 Caa (23) 38 Sr 66 Ba (17)	IIIB 21 Sc (74) 39 Y (120) 57-71 La-Lu	0 IVB 22 Ti (15) 40 Zr (38) 72 Hf (4)	SE(39) 2 VB 23 VB 23 V (32) 41 Nb (20) 7 3 Ta (18)	D6 78 11 VIB 24 Cr (118) 42 Mo (22) 74 W (11)	17 14 VIIB ²⁵ Mn ⁴³ Tc 75 Re (36)	3 26 Fe (203) 44 Ru (49) 76 Os (149)	VIIIB 27 Co (100) 45 Rh 77 Ir 62 Sm	VIIIB 28 Ni (227) 46 Pd (170) 78 Pt (242) 63 Eu	1B 29 Cu (23) 47 Ag (38) 79 Au (28)	11B 30 Zn (15) 48 Cd (18) B0 Hg (15)	111A 5 B (18) 13 AL (9) 31 Ca (14) 49 In (35) 81 TL (23) 66 Dy	IVA ⁶ C (18) ¹⁴ Si (29) ³² Cee (19) ⁵⁰ Sn (28) ⁸² Pb (66)	VA 7 N (11) 15 P (30) 33 As (20) 51 Sb (52) 83 Bi (49) 68 Er	VIA ⁸ O (27) ¹⁶ S (23) ³⁴ Se (37) ⁵² Te (42) ⁸⁴ Po ⁶⁹ Tm	VIIA 9 F (20) 17 Cl (18) 35 Br (20) 53 I (28) 85 At 70 Yb (100)	VIIIA ² He ¹⁰ Ne ⁽³³⁾ ¹⁸ Ar ⁽²⁷⁾ ³⁶ Kr ⁽²⁵⁾ ⁵⁴ Xe ⁽²¹⁾ ⁸⁶ Rn ⁷¹ Lu

Figure S6: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. Upper panel: HSE_{mix} calculations. Lower panel: PBE0 calculations. Gray cases indicate that there are no materials containing the corresponding element.

	IA																	VIIIA
1	1 H (9)	IIA	_	HS	SEn	nix							IIIA	IVA	VA	VIA	VIIA	² He
2	3 Li (36)	4 Be (15)		0	39	78 11	17 14	3					5 B (19)	6 C (18)	7 N (26)	8 0 (53)	9 F (20)	10 Ne (0)
3	11 Na (42)	12 Mg (18)	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	13 Al (13)	14 Si (25)	15 P (34)	16 S (32)	17 Cl (20)	18 Ar (15)
4	19 K (27)	20 Ca (28)	21 Sc (88)	22 Ti (51)	23 V (59)	24 Cr (140)	²⁵ Mn	26 Fe (282)	27 Co (241)	28 Ni (233)	29 Cu (35)	30 Zn (20)	31 Ga (18)	32 Ge (22)	33 As (28)	34 Se (42)	35 Br (23)	36 Kr (17)
5	37 Rb (34)	³⁸ Sr (40)	39 Y (123)	40 Zr (42)	41 Nb (43)	42 Mo (43)	⁴³ Tc	44 Ru (63)	⁴⁵ Rh	46 Pd (302)	47 Ag (53)	48 Cd (29)	49 In (48)	50 Sn (38)	51 Sb (61)	52 Te (48)	53 I (30)	54 Xe (15)
6	55 Cs (27)	56 Ba (19)	⁵⁷⁻⁷¹ La-Lu	72 Hf (15)	73 Ta (44)	74 W (21)	75 Re (45)	76 Os (151)	77 Ir	78 Pt (252)	79 Au (25)	80 Hg (32)	81 Tl (24)	82 Pb (87)	83 Bi (63)	⁸⁴ Po	⁸⁵ At	Rn
				57 La	⁵⁸ Ce	⁵⁹ Pr	60 Nd	61 Pm	⁶² Sm	Eu	G4 Gd	65 Tb	66 Dy	67 Ho	Er	⁶⁹ Tm	70 Yb	71 Lu
				(25) 89 Ac	90 Th	91 Pa	⁹² U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	¹⁰¹ Md	102 No	103 Lr
					(15)													
	IA																	VIIIA
1	1 1 (6)	IIA		Ρ	BE	0							IIIA	IVA	VA	VIA	VIIA	VIIIA ² He
1	IA 1 H (6) 3 Li (35)	4 Be (16)		P	BE	0 78 11	17 14	3					111A 5 B (18)	1VA 6 (28)	VA 7 N (32)	VIA 8 0 (42)	VIIA 9 F (19)	VIIIA ² He ¹⁰ Ne (30)
1 2 3	IA 1 H (6) 3 Li (35) 11 Na (43)	11A 4 Be (16) 12 Mg (39)	IIIB	Р 0 IVB	BE 39	0 78 11	17 14 VIIB	3 VIIIB	VIIIB	VIIIB	IB	IIB	111A 5 8 (18) 13 Al (15)	IVA ⁶ <u>C</u> (28) ¹⁴ <u>Si</u> (50)	VA 7 N (32) 15 P (55)	VIA 8 0 (42) 16 S (47)	VIIA 9 F (19) 17 CL (26)	VIIIA ² He ¹⁰ Ne ⁽³⁰⁾ ¹⁸ Ar ⁽²⁴⁾
1 2 3 4	IA 1 H (6) 3 Li (35) 11 Na (43) 19 K (36)	11A 4 Be (16) 12 Mg (39) 20 Ca (25)	111B 21 Sc (206)	P 0 IVB 22 Ti (36)	BE 39 7 VB	0 78 11 VIB 24 <u>Cr</u> (181)	VIIB 25 Mn	3 VIIIB 26 Fe (368)	VIIIB 27 Co (133)	VIIIB 28 Ni (690)	1B 29 Cu (44)	11B 30 Zn (47)	111A 5 8 (18) 13 AL (15) 31 Ca (31)	IVA ⁶ <u>C</u> (28) ¹⁴ <u>Si</u> (50) ³² <u>Ge</u> (44)	VA 7 N (32) 15 P (55) 33 As (65)	VIA ⁸ 0 (42) ¹⁶ S (47) ³⁴ Se (67)	VIIA 9 F (19) 17 CL (26) 35 Br (34)	VIIIA ² He ¹⁰ Ne ⁽³⁰⁾ ¹⁸ Ar ⁽²⁴⁾ ³⁶ Kr ⁽¹⁹⁾
1 2 3 4 5	IA 1 H (6) 3 Li (35) 11 Na (43) 19 K (36) 37 Rb (42)	11A 4 Be (16) 12 Mg (39) 20 Ca (25) 38 Sr (37)	111B 21 Sc (206) 39 Y (252)	P 0 IVB 22 Ti (36) 40 Zr (73)	BE 39 7 VB 23 V (68) 41 Nb (42)	0 78 1 VIB 24 Cr (181) 42 Mo (51)	VIIB 25 Mn 43 Tc	3 VIIIB 26 Fe (306) 44 Ru (131)	VIIIB 27 Co (133) 45 Rh	VIIIB 28 Ni (690) 46 Pd (366)	1B 29 Cu (44) (54)	11B 30 Zn (47) 48 Cd (50)	111A 5 B (18) 13 Al (15) 31 Ca (31) 49 In (68)	IVA ⁶ C (28) ¹⁴ Si (50) ³² Ge (44) ⁵⁰ Sn (57)	VA 7 N (32) 15 P (55) 33 As (65) 51 Sb (137)	VIA ⁸ 0 (42) ¹⁶ 5 6 6 7 7 7 7 7 7 7 7	VIIA 9 F (19) 17 Cl (26) 35 Br (34) 53 I (41)	VIIIA ² He ¹⁰ Ne (30) ¹⁸ Ar (24) ³⁶ Kr (19) ⁵⁴ Xe (15)
1 2 3 4 5 6	IA 1 H (6) 3 Li (35) 11 Na (43) 19 K (36) 37 Rb (42) 55 Cs (37)	11A 4 Be (16) 12 Mg (39) 20 Ca (25) 38 Sr (37) 56 Ba (37)	IIIB 21 Sc (206) 39 Y (252) 57-71 La-Lu	P 0 IVB 22 Ti (36) 40 Zr (73) 72 Hf (29)	BE 39 7 VB 23 V (68) 41 Nb (42) 73 Ta (47)	0 78 11 VIB 24 Cr (181) 42 Mo (51) 74 W (48)	VIIB 25 Mn 43 Tc 75 Re (83)	3 26 Fe (306) 44 Ru (131) 76 Os (272)	VIIIB 27 Co (133) 45 Rh 77 Ir	VIIIB 28 Ni (690) 46 Pd (306) 78 Pt (685)	1B 29 Cu (44) 47 Ag (54) 79 Au (27)	11B 30 Zn (47) 48 Cd (50) 80 Hg (42)	111A 5 8 (18) 13 AL (15) 31 Ga (31) 49 10 (68) 81 7 L (42)	IVA ⁶ <u>C</u> (28) ¹⁴ <u>Si</u> (50) ³² <u>Ge</u> (44) ⁵⁰ <u>Sn</u> (57) ⁸² <u>Pb</u>	VA 7 N (32) 15 P (55) 33 As (65) 51 Sb (137) 83 Bi (95)	VIA ⁸ 0 (42) 16 S (47) 34 Se (67) 52 Te (78) 84 Po	VIIA 9 F (19) 17 C(1 (26) 35 Br (34) 33 1 (41) 85 At	VIIIA ² He ¹⁰ Ne ⁽³⁰⁾ ¹⁸ Ar ⁽²⁴⁾ ³⁶ Kr ⁽¹⁹⁾ ⁵⁴ Xe ⁸⁶ Rn
1 2 3 4 5 6	IA 1 H (3) 11 Na (3) 19 K (36) 37 Rb (42) 55 Cs (37)	11A 4 Be (16) 12 Mg (39) 20 Ca (25) 38 Sr (37) 56 Ba (37)	IIIB 21 Sc (206) 39 Y (252) 57-71 La-Lu	P 0 IVB 22 Ti (36) 40 Zr (73) 72 Hf (29)	BE 39 VB 23 V (68) 41 Nb (42) 73 Ta (47)	0 78 1 VIB 24 Cr (181) 42 Mo (51) 74 W (48)	VIIB 25 Mn 43 Tc 75 Re (83) 60	3 VIIIB 26 Fe (368) 44 Ru (131) 76 Os (272)	VIIIB 27 Co (133) 45 Rh 77 Ir 62	VIIIB 28 Ni (690) 46 Pd (366) 78 Pt (685)	1B 29 Cu (44) (54) 79 Au (27) 64	11B 30 Zn (47) 48 Cd (50) 65	111A 5 B (18) 13 AI (15) 31 Ga (31) 49 In (68) 81 TL (42) 66	IVA ⁶ (28) ¹⁴ ⁵⁰ ³² Ge (44) ⁵⁰ ⁵⁰ ⁵⁰ ⁵⁷ ⁸² ^{Pb} ⁶⁷	VA 7 N (32) 15 P (55) 33 As (65) 15 Sb (137) 83 Bi (95) 15 15 15 15 15 15 15 15 15 15 15 15 15	VIA ⁸ 0 (42) ¹⁶ S (47) ³⁴ Se (67) ⁵² Te (78) ⁸⁴ Po	VIIA 9 F (19) 17 Cl (26) 35 Br (34) 53 l (41) 85 At (70)	VIIIA ² He ¹⁰ Ne ⁽³⁰⁾ ¹⁸ Ar ⁽²⁴⁾ ³⁶ Kr ⁽¹⁹⁾ ⁵⁴ Xe ⁽¹⁵⁾ ⁸⁶ Rn
1 2 3 4 5 6	IA 1 H (6) 3 Li (35) 11 Na (43) 19 K (36) 37 Rb (42) 55 Cs (37)	11A 4 Be (16) 12 Mg (39) 20 Ca (25) 38 Sr (37) 56 Ba (37)	111B 21 5c (206) 39 Y (252) 57-71 La-Lu	P 0 1VB 22 Ti (36) 40 Zr (73) 72 Hf (29) 57 La (28)	BE 39 ∶ ∨B 23 ∨ (68) 41 Nb (42) 73 Ta (47) 58 Ce	0 78 1 VIB 24 Cr (181) 42 Mo (51) 74 W (48) 59 Pr	VIIB 25 Mn 43 Tc 75 Re (83) 60 Nd	3 VIIIB 26 Fe (368) 44 Ru (131) 76 Os (272) 61 Pm	VIIIB 27 Co (133) 45 Rh 77 Ir 62 Sm	VIIIB 28 Ni (690) 46 Pd (366) 78 Pt (685) 63 Eu	IB 29 Cu (44) 47 Ag (54) 79 Au (27) 64 Gd	IIB 30 Zn (47) 48 Cd (50) 80 Hg (42) 65 Tb	111A 5 8 (18) 13 A1 (15) 31 Ga (31) 49 10 (68) 81 TL (42) 666 Dy	IVA ⁶ C (28) ¹⁴ Si ⁵⁰ Sn ⁽⁵⁷⁾ ⁸² Pb ⁽¹³⁹⁾ ⁶⁷ Ho	VA 7 N (32) 15 P (55) 33 As (65) 15 Sb (137) 83 Bi (95) 668 Er	VIA ⁸ 0 (42) ¹⁶ 5 (67) ⁵² Te (78) ⁸⁴ Po ⁶⁹ Tm	VIIA 9 F (19) 17 (26) 35 Br (34) 53 I (41) 85 At 70 Yb (90)	VIIIA ² He ¹⁰ Ne ⁽³⁰⁾ ¹⁸ Ar ⁽²⁴⁾ ³⁶ Kr ⁽¹⁹⁾ ⁵⁴ Xe ⁽¹⁵⁾ ⁸⁶ Rn ⁷¹ Lu

Figure S7: Mean absolute percentage error (in %) for the subsets of materials containing each element of the periodic table. $PBE0_{mix}$ calculations. Gray cases indicate that there are no materials containing the corresponding element.

1	A 1 (8)	IIA	l	PB	E0	mix							IIIA	IVA	VA	VIA	VIIA	VIIIA ² He
2	3 Li (44)	4 Be (15)		0	39 7	78 11	7 14	3					5 B (24)	6 C (17)	7 N (43)	8 (70)	9 F (30)	10 Ne (0)
3	11 Na (49)	12 Mg (30)	IIIB	IVB	VB	VIB	VIIB	VIIIB	VIIIB	VIIIB	IB	IIB	13 Al (16)	14 Si (23)	15 P (34)	16 S (42)	17 Cl (29)	18 Ar (8)
4	19 K (33)	20 Ca (35)	21 Sc (151)	22 Ti (68)	23 V (76)	24 Cr (121)	²⁵ Mn	26 Fe (173)	27 Co (262)	28 Ni (433)	29 Cu (43)	30 Zn (29)	31 Ga (27)	32 Ge (33)	33 As (36)	34 Se (51)	35 Br (31)	³⁶ Kr (10)
5	37 Rb (41)	38 Sr (53)	39 Y (166)	40 Zr (49)	41 Nb (58)	42 Mo (55)	⁴³ Tc	44 Ru (48)	⁴⁵ Rh	46 Pd (398)	47 Ag (71)	48 Cd (39)	49 In (59)	50 Sn (47)	51 Sb (80)	52 Te (55)	53 (35)	54 Xe (10)
6	55 Cs (35)	56 Ba (24)	57-71 La-Lu	72 Hf (22)	73 Ta (59)	74 W (31)	75 Re (48)	76 Os (109)	77 Ir	78 Pt (347)	79 Au (31)	80 Hg (45)	81 Tl (32)	82 Pb (128)	83 Bi (74)	⁸⁴ Po	⁸⁵ At	⁸⁶ Rn
				57 La (33)	⁵⁸ Ce	⁵⁹ Pr	⁶⁰ Nd	⁶¹ Pm	⁶² Sm	Eu	Gd ⁶⁴ Gd	⁶⁵ Tb	⁶⁶ Dу	67 Ho	Er	⁶⁹ Tm	70 Yb (91)	71 Lu
				⁸⁹ Ac	90 Th (18)	91 Pa	⁹² U	93 Np	⁹⁴ Pu	95 Am	96 Cm	97 Bk	⁹⁸ Cf	99 Es	¹⁰⁰ Fm	¹⁰¹ Md	102 No	¹⁰³ Lr



Figure S8: Histograms of MAPE and MPE for different functionals considered in this work as a function of the experimental band gap size. Due to the fact that few entries have band gap larger than 10 eV, all systems satisfying this condition are collected in one group. Figure S8: (cont.) Histograms of MAPE and MPE for different functionals considered in this work as a function of the experimental band gap size. Due to the fact that few entries have band gap larger than 10 eV, all systems satisfying this condition are collected in one group.



Figure S8: (cont.) Histograms of MAPE and MPE for different functionals considered in this work as a function of the experimental band gap size. Due to the fact that few entries have band gap larger than 10 eV, all systems satisfying this condition are collected in one group.



	LDA	LDA (SOC)	PBE	PBE (SOC)	PBEsol	HLE16	HLE16 (SOC)	BJ	mBJ	SCAN	HSE06	HSE14	$\mathrm{HSE}_{\mathrm{mix}}$	PBE0	PBE0 _{mix}
LDA		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LDA (SOC)			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE (SOC)					0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBEsol						0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HLE16							0.00	0.00	0.02	0.00	0.14	0.89	0.01	0.00	0.00
HLE16 (SOC)								0.00	0.02	0.00	0.21	0.90	0.03	0.00	0.00
BJ									0.00	0.03	0.00	0.00	0.00	0.89	0.88
mBJ										0.00	0.36	0.00	0.00	0.00	0.00
SCAN											0.00	0.00	0.00	0.66	0.60
HSE06												0.00	0.00	0.00	0.00
HSE14													0.00	0.00	0.00
$\mathrm{HSE06}_{\mathrm{mix}}$														0.00	0.00
PBE0															0.05
$\mathrm{PBE0_{mix}}$															

Table SI: Values of p obtained with the Wilcoxon signed-rank test for the absolute errors of each pair of functionals studied here. Due to the symmetry of the matix only the upper triangular part is shown. To improve readability, the statistic values W are not presented.

	LDA	LDA (SOC)	PBE	PBE (SOC)	PBEsol	HLE16	HLE16 (SOC)	BJ	mBJ	SCAN	HSE06	HSE14	$\mathrm{HSE}_{\mathrm{mix}}$	PBE0	$PBE0_{mix}$
LDA		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LDA (SOC)			0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PBE				0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.19	0.00
PBE (SOC)					0.33	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
PBEsol						0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00
HLE16							0.00	0.00	0.21	0.00	0.13	0.32	0.00	0.00	0.00
HLE16 (SOC)								0.00	0.46	0.00	0.19	0.22	0.00	0.00	0.00
BJ									0.00	0.10	0.00	0.00	0.02	0.00	0.04
mBJ										0.00	0.86	0.00	0.00	0.00	0.00
SCAN											0.00	0.00	0.00	0.00	0.19
HSE06												0.00	0.00	0.00	0.00
HSE14													0.00	0.00	0.00
$\mathrm{HSE06_{mix}}$														0.00	0.00
PBE0															0.00
$\mathrm{PBE0_{mix}}$															

Table SII: Values of p obtained with the Wilcoxon signed-rank test for the absolute percentage errors of each pair of functionals studied here. Due to the symmetry of the matix only the upper triangular part is shown. To improve readability, the statistic val