Supplementary information for: Hardness of Molecules and Bandgap of Solids from a Generalized Gradient Approximation Exchange Functional.

J. Carmona-Espíndola, Anaid Flores, José L. Gázquez, Alberto Vela, S. B. Trickey.

All properties included in the G3/99 test set were calculated at the equilibrium B3LYP/6-31G(2df,p) structures using B3LYP/6-31G(2df,p) zero-point energies obtained with a frequency scale factor of 0.9854.

The experimental or computational data were taken from the following references:

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Table S1: Mean absolute deviations (MAD) for NCAP and NCAPR functionals for several properties. Energies in kcal/mol, bond distances in $\AA$, frequencies in cm^{-1}, dipole moment in Debye and excited states in eV.

Property	NCAP	NCAPR
Heats of formation	5.97	7.33
Proton affinities	1.32	1.18
Binding energies	2.39	2.11
Barrier Heights	7.97	8.30
Bond distances	0.0251	0.0246
Frequencies	52.83	52.47
Dipole Moment	0.1430	0.1451
Excited States	0.44	0.60

Table S2: Mean absolute deviations (MAD) for different functionals for several properties. Energies in kcal/mol, bond distances in $\AA$, frequencies in cm^{-1}, dipole moment in Debye and excited states in eV.

Property	PBE	NCAPR	SCAN	PBE0	HSE06
Heats of formation	21.21	7.33	5.07	5.72	7.26
Proton affinities	1.39	1.18	1.28	1.16	1.05
Binding energies	1.64	2.11	1.56	1.05	1.00
Barrier Heights	9.89	8.30	8.57	5.46	4.80
Bond distances	0.0179	0.0246	0.0088	0.0103	0.0103
Frequencies	43.30	52.47	32.03	45.26	42.16
Dipole Moment	0.1529	0.1451	0.0892	0.0626	0.0618
Excited States	1.00	0.60	[a]	0.62	0.54

[a] Analytic second derivatives not ready for this XC functional in NWChem 6.5.

Table S3: Deviations of the standard enthalpies of formation for the molecules in the G3/99 set obtained with the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule	$\Delta_f H^o_{298}$	PBE	NCAPR	SCAN	PBE0	HSE06
1	LiH	33.3	5.0	0.6	3.0	5.8	5.5
2	BeH	81.7	-4.7	-6.9	-9.5	-5.0	-5.0
3	CH	142.5	-0.6	-3.0	2.3	1.2	1.6
4	$CH_2(^3B_1)$	93.7	-4.1	-5.5	-6.3	-3.3	-1.8
5	$CH_2(^1A_1)$	102.8	2.2	-1.4	5.8	4.9	6.1
6	CH_3	35.0	-2.5	-5.5	-4.7	-0.8	1.4
7	CH_4	-17.9	0.0	-3.9	0.7	2.5	5.7
8	NH	85.2	-4.5	-7.1	-0.8	-1.2	-0.8
9	NH_2	45.1	-6.1	-9.8	-1.8	-0.6	0.8
10	NH_3	-11.0	-2.9	-6.9	4.5	3.9	6.5
11	OH	9.4	-2.7	-3.8	-1.6	1.4	2.3
12	H_2O	-57.8	-0.4	-1.5	4.6	6.6	8.9
13	FH	-65.1	0.1	0.0	4.8	5.0	6.2
14	$SiH_2(^1A_1)$	65.2	3.5	-1.7	2.2	4.2	5.1
15	$SiH_2(^3B_1)$	86.2	-1.1	-4.7	-7.7	-1.6	-0.6
16	SiH_3	47.9	2.9	-3.6	-5.0	1.8	3.2
17	SiH_4	8.2	8.3	-0.4	-1.3	6.5	8.5
18	PH_2	33.1	-1.6	-6.7	-3.4	-0.0	1.1
19	PH_3	1.3	2.7	-4.0	0.7	4.6	6.5
20	H_2S	-4.9	0.5	-2.1	0.5	2.7	4.6
21	HCl	-22.1	0.1	-0.6	1.5	1.6	2.7
22	Li_2	51.6	4.6	6.0	6.3	5.4	5.4
23	LiF	-80.1	0.9	4.3	5.9	7.9	8.8
24	HCCH	54.2	-8.9	-3.0	4.1	1.4	5.6
25	CH_2CH_2	12.5	-8.1	-5.1	0.9	-0.3	5.2
26	CH_3CH_3	-20.1	-4.9	-4.7	-0.8	0.1	7.0
27	CN	104.9	-15.8	-9.9	4.4	3.0	5.3
28	HCN	31.5	-13.2	-8.2	5.8	2.0	5.2
29	CO	-26.4	-9.6	-2.4	5.2	4.0	6.8
30	CHO	10.0	-16.4	-9.9	-3.1	-1.6	1.9
31	CH_2O	-26.0	-12.0	-7.1	0.8	1.6	5.7
32	CH_3OH	-48.0	-6.9	-4.4	0.7	3.3	9.0
33	N_2	0.0	-14.7	-10.6	10.0	3.6	5.9

Table S3 – continued

34	N_2H_4	22.8	-13.4	-13.8	5.4	1.5	6.9
35	NO	21.6	-19.3	-13.6	2.0	-0.3	2.2
36	O_2	0.0	-23.6	-16.0	-7.2	-4.1	-1.1
37	H_2O_2	-32.5	-12.7	-8.4	2.3	6.1	10.6
38	F_2	0.0	-14.5	-8.7	1.1	3.2	5.5
39	CO_2	-94.1	-27.1	-11.9	-3.4	-2.2	3.3
40	Na_2	34.0	-0.7	2.7	2.7	1.2	1.0
41	Si_2	139.9	-6.7	-3.7	0.1	3.5	5.0
42	P_2	34.3	-4.2	-2.5	4.8	6.0	8.0
43	S_2	30.7	-13.7	-8.0	-7.8	-5.1	-2.6
44	Cl_2	0.0	-7.9	-2.3	-0.3	-1.6	0.6
45	NaCl	-43.6	4.1	6.4	2.2	4.9	5.8
46	SiO	-24.6	-3.2	1.6	5.9	10.2	12.7
47	CS	66.9	-8.3	-2.4	4.1	3.4	5.9
48	SO	1.2	-15.5	-8.9	-5.9	-1.1	1.6
49	ClO	24.2	-16.3	-10.3	-4.2	-2.0	0.4
50	ClF	-13.2	-10.7	-4.8	0.7	0.8	3.1
51	Si_2H_6	19.1	10.1	1.3	-5.9	7.5	12.0
52	CH_3Cl	-19.6	-5.5	-2.7	-1.3	-0.8	3.8
53	CH_3SH	-5.5	-4.7	-3.5	-1.2	0.6	6.0
54	HOCl	-17.8	-10.6	-5.6	0.6	2.1	5.5
55	SO_2	-71.0	-20.6	-7.0	-0.1	6.9	12.6
56	BF_3	-271.4	-11.0	9.0	0.3	4.2	10.7
57	BCl_3	-96.3	-13.6	5.1	-8.7	-6.9	-0.3
58	AlF_3	-289.0	0.6	15.7	5.6	14.8	19.7
59	$AlCl_3$	-139.7	-0.9	13.3	-6.1	0.5	5.8
60	CF_4	-223.0	-27.9	0.5	-4.9	-2.9	7.2
61	CCl4	-22.9	-21.5	4.1	-3.5	-5.9	3.8
62	COS	-33.1	-26.2	-12.3	-7.0	-5.0	0.3
63	CS_2	28.0	-23.8	-11.0	-8.5	-6.1	-1.3
64	COF_2	-149.1	-25.3	-3.6	-0.9	0.7	8.5
65	SiF_4	-386.0	2.3	24.5	8.4	19.1	27.2
66	SiCl4	-158.4	-3.6	18.0	-6.7	0.7	9.2
67	N_2O	19.6	-40.2	-28.1	-1.2	-4.8	0.2
68	NOCl	12.4	-33.3	-22.8	-4.8	-1.7	2.6
69	NF_3	-31.6	-40.3	-22.3	-6.2	-4.3	2.8
70	PF_3	-229.1	-10.3	6.0	4.1	9.5	16.2

Table S3 – continued

71	O_3	34.1	-37.8	-24.1	-1.1	7.3	12.7
72	F_2O	5.9	-30.6	-18.8	-4.6	1.2	5.8
73	ClF_3	-38.0	-39.5	-21.2	-11.7	-2.8	3.9
74	CF_2CF_2	-157.4	-47.3	-12.0	-12.8	-12.9	-0.6
75	CCl_2CCl_2	-3.0	-35.0	-1.3	-10.7	-13.9	-1.6
76	CF_3CN	-118.4	-41.9	-8.7	-1.7	-5.0	6.9
77	CH_3CCH(propyne)	44.2	-15.8	-5.6	0.8	-2.8	5.2
78	CH_2CCH_2(allene)	45.5	-20.6	-10.2	-3.1	-6.1	1.8
79	$C3H_4$(cyclopropene)	66.2	-18.7	-6.7	0.5	-5.8	2.8
80	CH_3CHCH_2(propylene)	4.8	-13.3	-5.8	-1.3	-2.8	6.6
81	$C3H_6$(cyclopropane)	12.7	-15.4	-5.9	-3.0	-6.3	3.8
82	$C3H_8$(propane)	-25.0	-9.0	-4.1	-2.1	-1.4	9.3
83	C_4H_6(1,3-butadien)	26.3	-22.2	-7.4	-2.6	-5.6	6.1
84	C_4H_6(2-butyne)	34.8	-21.7	-7.2	-1.5	-5.9	5.8
85	C_4H_6(methylene cyclopropane)	47.9	-28.0	-11.4	-6.9	-12.5	-0.1
86	C_4H_6(bicyclobutane)	51.9	-25.0	-6.1	-4.0	-10.9	2.4
87	C_4H_6(cyclobutene)	37.4	-22.7	-5.4	-2.4	-7.9	4.9
88	C_4H_8(cyclobutane)	6.8	-19.1	-4.7	-4.4	-7.7	6.5
89	C_4H_8(isobutene)	-4.0	-17.4	-4.9	-2.8	-4.2	9.1
90	C_4H_{10}(butane)	-30.0	-12.9	-3.4	-3.6	-2.8	11.7
91	C_4H_{10}(isobutane)	-32.1	-11.9	-2.0	-2.8	-1.8	12.9
92	C_5H_8(spiropentane)	44.3	-32.0	-8.8	-7.8	-15.6	1.5
93	C_6H_6(benzene)	19.7	-42.2	-9.0	-9.7	-18.1	0.2
94	CH_2F_2	-107.7	-14.4	-3.2	-1.6	0.0	6.3
95	CHF_3	-166.6	-21.3	-1.5	-3.1	-1.2	7.0
96	CH_2Cl_2	-22.8	-11.0	-0.9	-1.9	-3.1	3.1
97	$CHCl_3$	-24.7	-16.4	1.4	-2.8	-4.6	3.2
98	CH_3NH_2(methylamine)	-5.5	-8.1	-8.2	2.5	1.5	7.7
99	CH_3CN(acetronitrile)	18.0	-19.8	-10.6	2.8	-2.0	4.9
100	CH_3NO_2(nitromethane)	-17.8	-41.0	-24.2	-5.6	-4.1	5.8
101	CH_3ONO(methyl nitrite)	-15.9	-38.7	-22.9	-4.5	-1.4	8.5
102	CH_3SiH_3(methyl silane)	-7.0	5.2	0.8	-1.3	6.0	11.7
103	HCOOH(formic acid)	-90.5	-21.3	-8.6	-2.2	0.7	7.8
104	$HCOOCH_3$(methyl formate)	-85.0	-26.7	-10.0	-6.0	-1.5	9.3
105	CH_3CONH_2(acetamide)	-57.0	-26.9	-12.1	-2.9	-3.3	8.1
106	C_2H_4NH(aziridine)	30.2	-19.9	-11.2	-0.7	-5.3	3.9
107	C_2N_2(cyanogen)	73.3	-35.8	-17.9	6.4	-2.4	4.2

Table S3 – continued

108	$(CH_3)_2NH$(dimethylamine)	-4.4	-13.0	-8.5	0.4	-0.5	9.5
109	$CH_3CH_2NH_2$(ethylamine)	-11.3	-13.5	-8.9	-0.1	-1.2	8.8
110	CH_2CO(ketene)	-11.4	-25.7	-12.8	-5.0	-5.5	1.3
111	C_2H_4O(oxirane)	-12.6	-19.3	-8.4	-3.4	-3.4	5.3
112	CH_3CHO(acetaldehyde)	-39.7	-17.6	-8.0	-1.8	-1.1	6.9
113	HCOCHO(glyoxal)	-50.7	-29.7	-11.2	-1.8	-1.5	7.4
114	CH_3CH_2OH(ethanol)	-56.2	-11.1	-4.0	-0.8	1.7	11.2
115	CH_3OCH_3(dimethyl ether)	-44.0	-12.2	-5.4	-2.6	1.2	10.6
116	C_2H_4S(thiirane)	19.6	-16.4	-6.2	-4.4	-6.1	2.4
117	$(CH_3)_2SO$(dimethyl sulfoxide)	-36.2	-18.7	-5.7	-4.7	1.0	12.8
118	C_2H_5SH(ethanethiol)	-11.1	-8.5	-2.7	-1.9	-0.5	8.7
119	CH_3SCH_3(dimethyl sulfide)	-8.9	-9.8	-4.1	-2.9	-1.3	7.8
120	CH_2CHF(vinil fluoride)	-33.2	-17.9	-6.9	-3.0	-3.3	3.9
121	C_2H_5Cl(ethyl chloride)	-26.8	-9.7	-2.4	-2.4	-2.2	6.2
122	CH_2CHCl(vinyl chloride)	8.9	-18.5	-8.2	-5.6	-7.6	-0.5
123	CH_2CHCN(acrylonitrile)	43.2	-26.9	-10.7	3.7	-2.9	6.3
124	CH_3COCH_3(acetone)	-51.9	-21.8	-7.5	-3.6	-2.8	9.1
125	CH_3COOH(acetic acid)	-103.4	-25.2	-7.9	-3.9	-0.9	10.1
126	CH_3COF(acetyl fluoride)	-105.7	-25.3	-7.5	-4.2	-2.5	7.3
127	CH_3COCl(acetyl chloride)	-58.0	-25.4	-8.4	-5.9	-4.5	5.0
128	$CH_3CH_2CH_2Cl$(propyl chloride)	-31.5	-13.9	-2.0	-4.1	-3.9	8.4
129	$(CH_3)_2CHOH$(isopropanol)	-65.2	-14.8	-2.7	-2.2	0.6	14.2
130	$C_2H_5OCH_3$(methyl ethyl ether)	-51.7	-16.8	-5.4	-4.7	-0.8	12.5
131	$(CH_3)_3N$(trimethylamine)	-5.7	-17.5	-7.9	-1.9	-2.0	12.0
132	C_4H_4O(furan)	-8.3	-37.7	-9.6	-8.1	-11.8	2.9
133	C_4H_4S(thiophene)	27.5	-34.1	-6.9	-7.6	-13.3	1.2
134	C_4H_5N(pyrrole)	25.9	-39.3	-13.1	-6.1	-14.9	0.4
135	C_5H_5N(pyridine)	33.6	-47.6	-15.0	-8.4	-18.0	-0.6
136	H_2	0.0	4.9	-2.5	2.0	5.2	5.0
137	SH	34.2	-1.0	-2.6	-1.6	0.3	1.1
138	CCH(^2A',C_s)	135.1	-11.2	-4.2	0.1	-0.6	2.7
139	$CHCH_2$(^2A',C_s)	71.6	-13.1	-8.8	-5.7	-4.9	-0.2
140	CH_3CO(^2A',C_s)	-2.4	-22.2	-11.4	-5.8	-4.5	2.7
141	CH_2OH(^2A,C_1)	-4.1	-11.7	-7.7	-4.4	-0.9	4.1
142	CH_3O(^2A',C_s)	4.1	-12.4	-9.3	-6.6	-2.4	2.2
143	CH_3CH_2O(^2A",C_s)	-3.7	-18.4	-10.7	-9.2	-5.4	3.1
144	CH_3S(^2A',C_s)	29.8	-8.4	-6.0	-4.8	-3.4	1.1

Table S3 – continued

145	$CH_3CH_2(^2A'$,$C_s)$	28.9	-8.8	-7.5	-6.9	-4.0	2.0
146	$(CH_3)_2CH(^2A'$,$C_s)$	21.5	-14.5	-8.6	-9.0	-6.6	3.2
147	$(CH_3)_3C$(t-butyl radical C_{3v})	12.3	-18.5	-7.6	-9.8	-7.6	6.1
148	NO_2	7.9	-42.5	-29.0	-8.1	-6.1	-0.8
149	CH_2=C=$CHCH_3$ (1,2-butadiene)	38.8	-25.1	-10.4	-4.1	-7.9	3.8
150	CH_2=CH-C(CH_3)=CH_2 (isoprene)	18.0	-25.8	-5.8	-3.9	-6.6	9.1
151	C_5H_{10} (cyclopentane)	-18.3	-20.9	-1.1	-4.6	-7.8	10.7
152	C_5H_{12} (n-pentane)	-35.1	-16.6	-2.6	-4.6	-4.0	14.4
153	$C(CH_3)_4$ (neopentane)	-40.2	-13.6	1.7	-2.9	-1.1	17.8
154	C_6H_8 (1,3-cyclohexadiene)	25.4	-34.7	-4.5	-6.1	-12.8	6.9
155	C_6H_8 (1,4-cyclohexadiene)	25.0	-34.2	-4.1	-5.6	-12.8	6.9
156	C_6H_{12} (cyclohexane)	-29.5	-23.6	1.5	-6.4	-8.4	14.2
157	C_6H_{14} (n-hexane)	-39.9	-20.7	-2.0	-4.8	-5.5	16.7
158	C_6H_{14} (3-methyl pentane)	-41.1	-18.8	0.7	-4.8	-3.6	19.0
159	$C_6H_5CH_3$ (toluene)	12.0	-46.3	-8.3	-11.3	-19.4	2.8
160	C_7H_{16} (n-heptane)	-44.9	-24.5	-1.2	-7.0	-6.8	19.3
161	C_8H_8 (1,3,5,7-cyclooctatetraene)	70.7	-51.8	-6.7	-6.7	-17.9	6.7
162	C_8H_{18} (n-octane)	-49.9	-28.4	-0.5	-9.0	-8.1	21.8
163	$C_{10}H_8$ (naphthalene)	35.9	-75.4	-11.6	-19.8	-34.2	-3.0
164	$C_{10}H_8$ (azulene)	69.1	-78.2	-14.8	-19.2	-33.0	-2.4
165	CH_3COOCH_3 (methyl acetate)	-98.4	-29.5	-8.2	-6.8	-2.1	12.6
166	$(CH_3)_3COH$ (t-butanol)	-74.7	-17.2	0.2	-3.0	0.7	18.4
167	$C_6H_5NH_2$ (aniline)	20.8	-52.6	-14.4	-11.1	-20.6	1.0
168	C_6H_5OH (phenol)	-23.0	-50.2	-9.4	-11.6	-17.5	3.7
169	CH_2=CH-O-CH=CH_2 (divinyl ether)	-3.3	-31.6	-9.7	-5.3	-5.9	8.5
170	C_4H_8O (tetrahydrofuran)	-44.0	-24.4	-2.8	-5.5	-5.5	11.7
171	C_5H_8O (cyclopentanone)	-45.9	-35.4	-6.2	-8.0	-10.9	8.7
172	$C_6H_4O_2$ (1,4-benzoquinone)	-29.4	-60.9	-12.3	-9.9	-14.8	6.8
173	$C_4H_4N_2$ (pyrimidine)	46.8	-54.1	-22.2	-8.4	-19.5	-2.9
174	$(CH_3)_2SO_2$ (dimethyl sulfone)	-89.2	-23.7	-2.5	-7.3	3.0	18.0
175	C_6H_5Cl (chlorobenzene)	12.4	-48.2	-7.5	-11.9	-20.9	-1.0
176	NC-CH_2CH_2-CN (succinonitrile)	50.1	-42.1	-15.2	5.3	-6.2	8.2
177	$C_4H_4N_2$ (pyrazine)	46.9	-50.5	-18.7	-4.2	-15.3	1.2
178	CH_3COCCH (acetyl acetylene)	15.6	-31.0	-7.1	-0.2	-2.7	10.0
179	CH_3-CH=CH-CHO (crotonaledehyde)	-24.0	-32.8	-11.4	-6.5	-7.5	6.7
180	$(CH_3CO)_2O$ (acetic anhydride)	-136.8	-48.5	-13.1	-10.7	-6.7	13.0
181	C_4H_6S (25-dihydrothiophene)	20.8	-27.5	-4.2	-5.8	-10.3	5.2

Table S3 – continued

182	$CH_3CH(CH_3)CN$ (2-methyl propanenitrile)	5.6	-25.3	-6.9	2.4	-2.5	12.1
183	CH_3-CO-CH_2CH_3 (methyl ethyl ketone)	-57.1	-25.7	-6.7	-5.4	-4.2	11.6
184	$(CH_3)_2$CH-CHO (isobutyraldehyde)	-51.6	-23.7	-4.7	-2.7	-2.1	13.6
185	$C_4H_8O_2$ (1,4-dioxane)	-75.5	-31.8	-3.0	-8.7	-4.4	15.6
186	C_4H_8S (tetrahydrothiophene)	-8.2	-21.0	-0.3	-5.0	-7.0	10.0
187	$(CH_3)_3$C-Cl (t-butyl chloride)	-43.5	-15.7	1.9	-4.6	-3.0	13.5
188	$CH_3CH_2CH_2CH_2Cl$ (n-butyl chloride)	-37.0	-17.2	-0.6	-3.8	-4.6	11.5
189	C_4H_8NH (pyrrolidine)	-0.8	-25.8	-6.4	-3.2	-7.7	10.0
190	$CH_3CH_2CH(NO_2)CH_3$ (2-nitrobutane)	-39.1	-51.4	-20.1	-9.3	-7.0	14.8
191	$CH_3CH_2OCH_2CH_3$ (diethyl ether)	-60.3	-20.4	-4.4	-5.1	-1.8	15.3
192	CH_3-$CH(OCH_3)_2$ (1,1-dimethoxy ethane)	-93.1	-21.8	1.4	-1.7	5.1	25.1
193	$(CH_3)_3$C-SH (t-butanethiole)	-26.2	-14.4	1.9	-3.8	-1.2	16.3
194	$(CH_3CH_2S)_2$ (diethyl disulfide)	-17.9	-22.5	-2.2	-7.6	-4.3	14.7
195	$(CH_3)_3$C-NH_2 (t-butylamine)	-28.9	-18.2	-3.2	-1.0	-0.9	17.2
196	$Si(CH_3)_4$ (tetramethyl silane)	-55.7	-1.9	7.6	-0.4	6.7	23.8
197	C_5H_6S (2-methyl thiopehene)	20.0	-38.4	-6.6	-8.8	-14.9	3.4
198	C_5H7N (N-methyl pyrrole)	24.6	-43.2	-12.6	-7.9	-15.9	3.2
199	$C_5H_{10}O$ (tetrahydropyran)	-53.4	-27.5	-0.5	-7.4	-6.3	15.1
200	$C_2H_5COC_2H_5$ (diethyl ketone)	-61.6	-30.3	-6.5	-7.4	-6.3	13.4
201	$CH_3COOCH(CH_3)_2$ (isopropyl acetate)	-115.1	-36.7	-5.7	-8.4	-4.2	18.4
202	$C_5H_{10}S$ (tetrahydrothiopyran)	-15.2	-24.5	1.6	-6.6	-8.1	13.1
203	$C_5H_{10}NH$ (piperidine)	-11.3	-28.8	-4.0	-5.1	-8.6	13.4
204	$(CH_3)_3COCH_3$ (t-butyl methyl ether)	-67.8	-21.4	0.6	-5.8	-0.3	21.3
205	$C_6H_4F_2$ (1,3-difluuorobenzene)	-73.9	-59.6	-10.1	-15.8	-22.1	-0.3
206	$C_6H_4F_2$ (1,4-difluuorobenzene)	-73.3	-59.5	-10.0	-15.6	-21.9	-0.2
207	C_6H_5F (fluorobenzene)	-27.7	-50.6	-9.3	-12.4	-19.8	0.2
208	$(CH_3)_2CHOCH(CH_3)_2$ (diisopropyl ether)	-76.3	-26.2	0.0	-6.5	-2.4	22.8
209	PF_5	-381.1	-10.6	20.1	4.2	14.8	26.7
210	SF_6	-291.7	-32.4	9.8	-9.8	5.6	21.4
211	P_4	14.1	-19.5	-5.2	-2.6	-3.3	4.3
212	SO_3	-94.6	-30.6	-9.2	-5.0	5.3	13.8
213	SCl_2	-4.2	-14.8	-3.8	-4.6	-3.7	0.7
214	$POCl_3$	-133.8	-17.5	5.3	-7.3	1.3	10.5
215	PCl_5	-86.1	-21.9	6.8	-14.2	-5.9	5.6
216	SO_2Cl_2	-84.8	-31.5	-4.9	-10.8	0.6	10.8
217	PCl_3	-69.0	-14.7	0.3	-6.3	-2.7	3.5
218	S_2Cl_2	-4.0	-27.5	-11.0	-12.7	-9.0	-2.6

Table S3 – continued

219	$SiCl_2$ ($^1A_1$)	-40.3	-5.9	3.5	-2.6	0.2	4.1
220	CF_3Cl	-169.5	-28.4	-0.7	-6.7	-4.9	5.1
221	C_2F_6	-321.3	-46.6	2.6	-10.6	-6.0	11.4
222	CF_3	-111.3	-28.6	-7.5	-9.7	-7.2	0.1
223	C_6H_5 (phenyl radical)	81.2	-47.8	-13.4	-16.4	-22.9	-5.4

Table S4: Deviations of the ionization potential for the test set IP13/3 for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	C	259.7	6.3	6.0	9.7	5.7	5.9
2	S	238.9	0.4	3.5	-0.4	-0.2	0.2
3	SH	238.9	-0.4	1.6	-0.1	-0.8	-0.6
4	Cl	299.1	0.2	1.8	1.4	-0.1	0.0
5	Cl_2	265.3	-4.2	-2.5	1.2	0.7	0.8
6	OH	299.1	4.2	5.9	2.2	0.6	1.0
7	O	313.9	10.2	13.4	3.4	5.5	6.3
8	O_2	278.9	7.0	8.3	14.0	11.2	11.6
9	P	241.9	0.4	0.2	3.7	1.4	1.3
10	PH	234.1	2.5	2.7	6.5	3.5	3.5
11	PH_2	226.3	3.8	4.3	8.5	4.8	4.8
12	S_2	216.0	4.2	5.2	9.2	8.4	8.5
13	Si	187.9	1.3	1.8	4.1	1.7	1.8

Table S5: Deviations of the electron affinities for the test set EA13/3 for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	C	29.1	7.0	7.1	4.6	3.4	3.1
2	S	47.9	1.8	4.0	1.2	-0.3	-0.3
3	SH	53.3	0.4	1.7	-1.4	-1.4	-1.6
4	Cl	83.4	1.7	2.9	1.2	0.1	-0.0
5	Cl_2	55.6	12.2	15.1	14.3	11.8	12.8
6	OH	42.1	0.5	1.7	-6.8	-6.7	-6.7
7	O	33.7	5.1	7.0	0.0	-2.7	-2.5
8	O_2	10.8	-0.3	2.2	-3.5	-3.5	-3.0
9	P	17.2	1.7	5.4	-0.3	-0.5	-0.3
10	PH	23.2	0.2	2.5	-1.7	-1.9	-1.9
11	PH_2	29.4	-1.4	0.0	-4.0	-3.2	-3.3
12	S_2	38.5	-0.1	1.9	-0.4	0.8	0.9
13	Si	31.9	2.0	2.7	3.2	1.5	1.3

Table S6: Deviations of the proton affinities for the test set PA8 for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	NH_3	211.9	-1.3	0.1	0.0	0.6	0.9
2	H_2O	171.8	-2.0	-0.7	-0.7	-0.3	-0.1
3	HCCH	156.6	2.6	4.2	4.0	3.9	4.3
4	SiH_4	156.5	-0.9	1.5	-2.4	-1.8	-0.8
5	PH_3	193.1	-2.6	-0.5	-0.4	-0.5	0.2
6	H_2S	173.7	-0.2	1.5	-0.0	0.1	0.7
7	HCl	137.1	-0.7	0.8	-1.4	-1.2	-0.7
8	H_2	105.9	-0.9	0.1	-1.4	-0.9	-0.7

Table S7: Deviations of the binding energies for the 31 weakly interacting systems for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	$(NH_3)_2$	3.15	1.08	-0.90	1.21	0.92	0.58
2	$(HF)_2$	4.57	0.73	-1.37	1.25	0.65	0.32
3	$(H_2O)_2$	4.97	1.56	-0.67	1.86	1.50	1.07
4	NH_3-H_2O	6.41	2.23	-0.10	2.11	1.96	1.45
5	$(HCONH_2)_2$	14.94	-0.20	-4.09	1.18	-0.07	-1.20
6	$(HCOOH)_2$	16.15	0.62	-3.59	2.05	0.97	-0.38
7	C_2H_4-F2	1.06	2.30	0.19	1.98	0.52	0.38
8	NH_3-F2	1.81	4.66	2.33	3.65	1.77	1.54
9	C_2H_2-ClF	3.81	2.31	-0.29	3.36	0.72	0.08
10	HCN-ClF	4.86	1.09	-1.44	0.72	0.16	-0.43
11	NH_3-Cl2	4.88	4.89	2.32	4.10	2.84	2.24
12	H_2O-ClF	5.36	2.98	0.29	3.41	1.75	1.11
13	NH_3-ClF	10.62	8.09	4.65	7.99	4.75	3.76
14	$(H_2S)_2$	1.66	0.53	-1.16	-1.40	0.32	0.03
15	$(HCl)_2$	2.01	0.25	-1.50	0.75	0.03	-0.28
16	HCl-H_2S	3.35	1.29	-0.69	0.53	0.84	0.41
17	CH_3Cl-HCl	3.55	0.02	-2.40	1.85	-0.28	-0.81
18	HCN-CH_3SH	3.59	0.12	-2.09	0.90	-0.02	-0.42
19	CH_3SH-HCl	4.16	2.00	-0.66	2.33	1.40	0.75
20	HeNe	0.04	0.28	-0.37	0.18	0.18	0.18
21	HeAr	0.06	0.40	-0.36	0.67	0.25	0.25
22	Ne_2	0.08	0.15	-0.72	0.19	0.08	0.09
23	NeAr	0.13	0.06	-0.92	0.14	-0.01	-0.02
24	CH_4-Ne	0.22	0.08	-1.03	0.34	-0.00	-0.01
25	C_6H_6-Ne	0.47	-0.08	-2.13	0.22	-0.20	-0.30
26	$(CH_4)_2$	0.51	-0.50	-2.23	0.09	-0.54	-0.71
27	$(C_2H_2)_2$	1.34	-0.24	-1.89	-0.55	-0.29	-0.47
28	$(C_2H_4)_2$	1.42	-0.91	-3.44	-0.85	-0.93	-1.31
29	Sandwich C_6H_6	1.81	-3.80	-7.26	-0.97	-3.14	-3.63
30	T-Shaped C_6H_6	2.74	-2.97	-6.09	0.59	-1.98	-2.55
31	Parallel C_6H_6	2.78	-4.30	-8.15	-1.03	-3.46	-4.18

Table S8: Deviations of the FORWARD barrier heights of hydrogen transfer reactions for the HTBH38/04 test set for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	$H + HCl \rightarrow H_2 + Cl$	5.7	-5.2	-7.9	-7.5	-2.8	-2.8
2	$OH + H_2 \rightarrow H + H_2O$	5.7	-11.5	-7.3	-7.5	-5.3	-3.9
3	$CH_3 + H_2 \rightarrow H + CH_4$	12.1	-8.2	-4.2	-4.9	-5.1	-3.9
4	$OH + CH_4 \rightarrow CH_3 + H_2O$	6.7	-11.8	-7.9	-8.0	-4.6	-3.3
5	$H + H_2 \rightarrow H_2 + H$	9.6	-5.9	-7.1	-7.2	-3.9	-3.5
6	$OH + NH_3 \rightarrow H_2O + NH_2$	3.2	-15.3	-11.2	-10.6	-5.4	-4.2
7	$HCl + CH_3 \rightarrow Cl + CH_4$	1.7	-7.5	-4.2	-4.7	-3.9	-2.9
8	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	3.4	-11.9	-7.8	-8.0	-4.1	-2.9
9	$F + H_2 \rightarrow HF + H$	1.8	-13.7	-10.1	-8.9	-5.9	-4.9
10	$O + CH_4 \rightarrow OH + CH_3$	13.7	-13.5	-10.2	-11.2	-5.5	-4.5
11	$H + PH_3 \rightarrow PH_2 + H_2$	3.1	-4.8	-6.2	-6.1	-2.6	-2.4
12	$H + HO \rightarrow H_2 + O$	10.7	-7.3	-9.3	-7.6	-3.8	-3.7
13	$H + H_2S \rightarrow H_2 + HS$	3.5	-4.7	-6.0	-6.3	-2.3	-2.1
14	$O + HCl \rightarrow OH + Cl$	9.8	-20.2	-16.2	-14.0	-7.3	-6.2
15	$NH_2 + CH_3 \rightarrow CH_4 + NH$	8.0	-7.6	-4.0	-3.6	-3.1	-2.0
16	$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$	7.5	-4.9	-1.2	-1.6	-0.7	0.4
17	$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$	10.4	-8.9	-4.6	-5.7	-3.0	-1.7
18	$NH_2 + CH_4 \rightarrow CH_3 + NH_3$	14.5	-10.1	-6.1	-6.8	-4.5	-3.2
19	$C_5H_8 \rightarrow C_5H_8$	38.4	-7.2	-4.9	-4.6	-2.8	-1.7

Table S9: Deviations of the BACKWARD barrier heights of hydrogen transfer reactions for the HTBH38/04 test set for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	$H + HCl \rightarrow H_2 + Cl$	8.7	-9.8	-5.7	-7.9	-6.2	-4.9
2	$OH + H_2 \rightarrow H + H_2O$	21.2	-8.0	-11.1	-10.5	-4.3	-4.5
3	$CH_3 + H_2 \rightarrow H + CH_4$	15.3	-5.9	-8.4	-8.3	-3.3	-3.3
4	$OH + CH_4 \rightarrow CH_3 + H_2O$	19.6	-11.2	-8.1	-8.3	-6.0	-5.0
5	$H + H_2 \rightarrow H_2 + H$	9.6	-5.9	-7.1	-7.2	-3.9	-3.5
6	$OH + NH_3 \rightarrow H_2O + NH_2$	12.7	-14.2	-10.2	-10.0	-5.8	-4.6
7	$HCl + CH_3 \rightarrow Cl + CH_4$	7.9	-9.7	-6.3	-8.5	-5.5	-4.3
8	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	19.9	-9.6	-6.5	-7.4	-4.6	-3.7
9	$F + H_2 \rightarrow HF + H$	33.4	-9.1	-12.9	-11.9	-5.9	-6.4
10	$O + CH_4 \rightarrow OH + CH_3$	8.1	-8.9	-5.4	-4.9	-4.3	-3.2
11	$H + PH_3 \rightarrow PH_2 + H_2$	23.2	-4.9	-0.3	-3.6	-2.7	-1.3
12	$H + HO \rightarrow H_2 + O$	13.1	-14.1	-9.8	-10.5	-6.9	-5.5
13	$H + H_2S \rightarrow H_2 + HS$	17.3	-7.8	-2.7	-6.0	-4.9	-3.3
14	$O + HCl \rightarrow OH + Cl$	10.4	-18.0	-13.6	-11.6	-7.7	-6.4
15	$NH_2 + CH_3 \rightarrow CH_4 + NH$	22.4	-11.5	-8.3	-9.9	-5.6	-4.6
16	$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$	18.3	-10.5	-6.9	-8.8	-4.2	-3.1
17	$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$	17.4	-7.7	-4.3	-5.6	-3.0	-2.0
18	$NH_2 + CH_4 \rightarrow CH_3 + NH_3$	17.8	-10.5	-7.1	-7.6	-5.5	-4.4
19	$C_5H_8 \rightarrow C_5H_8$	38.4	-7.2	-4.9	-4.6	-2.8	-1.7

Table S10: Deviations of the FORWARD barrier heights of non-hydrogen transfer reactions for the NHTBH38/04 test set for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	$H + N_2O \rightarrow OH + N_2$	18.14	-7.66	-8.65	-8.37	-3.75	-3.25
2	$H + FH \rightarrow HF + H$	42.18	-14.24	-14.23	-12.57	-7.47	-6.89
3	$H + ClH \rightarrow + HCl\ H$	18.00	-8.31	-8.86	-8.91	-4.52	-3.95
4	$H + FCH_3 \rightarrow HF + CH_3$	30.38	-11.13	-12.76	-9.70	-4.04	-3.94
5	$H + F_2 \rightarrow HF + F$	2.27	35.65	34.34	35.91	45.57	45.73
6	$CH_3 + FCl \rightarrow CH_3F + Cl$	7.43	-12.96	-10.57	-11.41	-5.62	-5.27
7	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-14.16	-10.89	-13.31	-7.22	-6.45
8	$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	13.38	-7.75	-7.76	-7.11	-2.98	-2.79
9	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.10	-9.68	-7.43	-9.59	-4.44	-4.06
10	$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	13.61	-7.43	-7.74	-6.73	-3.18	-3.23
11	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	-12.54	-14.10	-11.33	-15.18	-8.32	-7.69
12	$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	2.89	-5.30	-5.67	-6.53	-2.78	-2.75
13	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	-2.78	-14.35	-10.89	-13.26	-7.68	-6.92
14	$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	10.96	-10.56	-10.29	-9.31	-5.01	-4.84
15	$H + N_2 \rightarrow HN_2$	14.69	-9.38	-10.18	-10.38	-6.03	-5.47
16	$H + CO \rightarrow HCO$	3.17	-4.90	-5.64	-6.84	-2.88	-2.44
17	$H + C2H_4 \rightarrow CH_3CH_2$	1.72	-1.83	-2.86	-6.19	-1.00	-0.60
18	$CH_3 + C2H_4 \rightarrow CH_3CH_2CH_2$	6.85	-5.28	-1.64	-6.19	-2.70	-1.57
19	$HCN \rightarrow HNC$	48.16	-2.46	-2.41	-1.72	-1.71	-1.46

Table S11: Deviations of the BACKWARD barrier heights of non-hydrogen transfer reactions for the NHTBH38/04 test set for the exchange-correlation functional shown in each column. All quantities are in kcal/mol.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	$H + N_2O \rightarrow OH + N_2$	83.22	-30.94	-22.85	-18.60	-14.27	-12.05
2	$H + FH \rightarrow HF + H$	42.18	-14.24	-14.23	-12.57	-7.47	-6.89
3	$H + ClH \rightarrow HCl + H$	18.00	-8.31	-8.86	-8.91	-4.52	-3.95
4	$H + FCH_3 \rightarrow HF + CH_3$	57.02	-15.83	-11.20	-10.36	-6.82	-5.63
5	$H + F_2 \rightarrow HF + F$	106.18	19.56	24.04	30.76	42.62	43.75
6	$CH_3 + FCl \rightarrow CH_3F + Cl$	60.17	-18.67	-16.55	-14.65	-6.86	-6.56
7	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-14.16	-10.89	-13.31	-7.22	-6.45
8	$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	13.38	-7.75	-7.76	-7.11	-2.98	-2.79
9	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.10	-9.68	-7.43	-9.59	-4.44	-4.06
10	$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	13.61	-7.43	-7.74	-6.73	-3.18	-3.23
11	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	20.11	-8.19	-5.27	-5.19	-0.95	-0.46
12	$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	29.62	-6.89	-6.60	-4.03	-0.25	-0.18
13	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	17.33	-14.21	-11.24	-13.26	-6.05	-5.35
14	$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	47.20	-2.86	-4.29	-2.40	2.82	2.40
15	$H + N_2 \rightarrow HN_2$	10.72	-1.93	-1.71	-1.20	0.69	0.58
16	$H + CO \rightarrow HCO$	22.68	1.73	1.74	1.31	2.61	2.42
17	$H + C_2H_4 \rightarrow CH_3CH_2$	41.75	-1.41	-0.73	1.41	2.50	2.44
18	$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	32.97	-3.05	-5.20	-2.02	1.60	0.72
19	$HCN \rightarrow HNC$	33.11	-2.38	-2.28	-0.76	-0.34	-0.21

Table S12: Deviations of the bond lengths for the test set T96-R for the exchange-correlation functional shown in each column. All quantities are in $\mathring{A}$.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	H_2	0.741	0.010	0.008	0.001	0.004	0.003
2	Li_2	2.673	0.065	0.079	0.082	0.063	0.066
3	LiH	1.595	0.012	0.015	0.007	0.004	0.004
4	LiF	1.564	0.012	0.025	0.005	-0.000	0.002
5	LiCl	2.021	0.004	0.021	0.006	-0.003	-0.000
6	LiO	1.688	0.011	0.024	0.005	-0.005	-0.002
7	Be2	2.440	0.001	0.034	0.046	0.078	0.076
8	BeH	1.343	0.019	0.019	0.011	0.012	0.011
9	BeF	1.361	0.019	0.026	0.009	0.007	0.009
10	BeO	1.331	0.015	0.018	0.001	-0.007	-0.006
11	BeS	1.742	0.015	0.020	0.001	-0.001	0.000
12	B_2	1.590	0.029	0.036	0.028	0.024	0.025
13	BH	1.232	0.020	0.021	0.009	0.009	0.008
14	BF	1.263	0.013	0.019	0.002	0.000	0.001
15	BF_3	1.313	0.012	0.018	-0.001	-0.002	-0.000
16	BCl	1.715	0.016	0.026	0.004	0.003	0.005
17	BCl_3	1.742	0.006	0.015	-0.003	-0.005	-0.002
18	BN	1.281	0.051	0.056	0.038	0.034	0.035
19	BO	1.204	0.010	0.014	0.000	-0.004	-0.003
20	BS	1.609	0.012	0.016	0.001	-0.002	-0.000
21	C_2	1.242	0.162	0.167	0.006	0.004	0.005
22	CH	1.120	0.017	0.018	0.005	0.005	0.005
23	CH_4	1.087	0.009	0.010	0.001	0.002	0.002
24	CF	1.272	0.015	0.022	0.003	-0.004	-0.002
25	CF_4	1.323	0.015	0.021	-0.001	-0.005	-0.003
26	CCl	1.645	0.015	0.025	0.006	-0.000	0.003
27	CCl_4	1.767	0.015	0.026	0.003	-0.004	-0.000
28	CN	1.172	0.002	0.006	-0.009	-0.012	-0.011
29	CO	1.128	0.008	0.011	-0.002	-0.005	-0.004
30	CO^+	1.115	0.007	0.010	-0.005	-0.009	-0.008
31	CO_2	1.160	0.011	0.014	-0.001	-0.003	-0.002
32	CP	1.562	0.005	0.009	-0.010	-0.012	-0.011
33	CS	1.535	0.011	0.016	-0.001	-0.006	-0.004
34	CS_2	1.553	0.009	0.014	-0.002	-0.005	-0.003
35	N_2	1.098	0.005	0.007	-0.006	-0.009	-0.008
36	N_2^+	1.116	-0.002	0.001	-0.011	-0.014	-0.013
37	NH	1.036	0.015	0.016	0.004	0.002	0.002
38	NH^+	1.070	0.021	0.022	0.007	0.006	0.006
39	NF	1.317	0.010	0.019	-0.001	-0.014	-0.011
40	NCl	1.611	0.007	0.018	0.004	-0.006	-0.003
41	NO	1.151	0.007	0.011	-0.004	-0.011	-0.010
42	NO^+	1.063	0.007	0.009	-0.005	-0.009	-0.009
43	NS	1.494	0.012	0.017	-0.002	-0.009	-0.007
44	O_2	1.208	0.011	0.016	-0.002	-0.015	-0.014
45	O_2^+	1.116	0.006	0.010	-0.007	-0.018	-0.017
46	OH	0.970	0.013	0.015	0.002	0.001	0.001
47	OH^+	1.029	0.019	0.019	0.005	0.003	0.003
48	OF	1.358	0.001	0.011	-0.007	-0.028	-0.025
49	F_2	1.412	0.002	0.011	-0.012	-0.036	-0.033
50	F_2^+	1.322	-0.006	0.001	-0.024	-0.049	-0.047
51	HF	0.917	0.013	0.014	0.003	0.001	0.001

Table S12 – continued

52	HF^+	1.001	0.022	0.022	0.008	0.006	0.006
53	Na_2	3.079	0.000	0.043	0.043	0.005	0.032
54	NaH	1.887	0.006	0.018	0.006	0.000	0.005
55	NaF	1.926	0.016	0.029	-0.002	-0.002	0.003
56	NaCl	2.361	0.009	0.030	0.000	-0.000	0.005
57	NaO	2.052	0.020	0.034	0.000	-0.003	0.002
58	MgH	1.730	0.027	0.030	0.013	0.014	0.015
59	MgF	1.750	0.032	0.040	0.012	0.012	0.016
60	MgCl	2.196	0.029	0.041	0.012	0.014	0.018
61	MgO	1.748	0.002	0.010	-0.015	-0.016	-0.012
62	Al_2	2.466	0.023	0.039	0.009	0.013	0.017
63	AlH	1.648	0.032	0.033	0.013	0.017	0.017
64	AlF	1.654	0.028	0.036	0.007	0.008	0.011
65	AlCl	2.130	0.032	0.043	0.012	0.015	0.019
66	AlO	1.618	0.014	0.020	-0.001	-0.000	0.002
67	AlS	2.029	0.020	0.028	-0.000	0.002	0.005
68	Si_2	2.246	0.040	0.048	-0.096	-0.098	-0.094
69	SiH	1.520	0.025	0.027	0.009	0.012	0.012
70	SiH_4	1.480	0.013	0.014	0.001	0.005	0.005
71	SiF	1.601	0.032	0.038	0.011	0.010	0.013
72	SiF_4	1.553	0.028	0.033	0.009	0.009	0.011
73	SiCl	2.058	0.027	0.038	0.011	0.010	0.014
74	SiCl	2.019	0.021	0.030	0.004	0.004	0.007
75	SiN	1.572	0.007	0.012	-0.005	-0.009	-0.007
76	SiO	1.510	0.019	0.023	0.003	-0.002	-0.001
77	SiS	1.929	0.022	0.028	0.004	0.001	0.003
78	P_2	1.893	0.013	0.017	-0.005	-0.011	-0.009
79	P_4	2.210	-0.001	0.008	-0.014	-0.026	-0.022
80	PH	1.421	0.020	0.021	0.005	0.007	0.008
81	PF	1.589	0.029	0.036	0.009	0.005	0.008
82	PCl	2.015	0.017	0.027	0.004	-0.000	0.004
83	PN	1.491	0.008	0.012	-0.006	-0.012	-0.011
84	PO	1.476	0.021	0.025	0.003	-0.002	-0.001
85	S_2	1.889	0.022	0.030	0.006	-0.003	0.000
86	SH	1.341	0.016	0.017	0.004	0.005	0.005
87	SF	1.601	0.022	0.030	0.002	-0.006	-0.003
88	SF_6	1.561	0.036	0.044	0.013	0.004	0.007
89	SO	1.481	0.024	0.030	0.005	-0.002	0.000
90	SO_3	1.420	0.024	0.029	0.004	-0.001	0.001
91	Cl_2	1.988	0.017	0.031	0.009	-0.008	-0.003
92	Cl_2^+	1.891	0.023	0.033	0.008	-0.008	-0.004
93	HCl	1.275	0.014	0.015	0.004	0.003	0.004
94	HCl^+	1.315	0.018	0.019	0.006	0.006	0.006
95	ClF	1.628	0.023	0.034	0.005	-0.009	-0.005
96	ClO	1.570	0.013	0.023	0.007	-0.009	-0.005

Table S13: Deviations of the harmonic vibrational frequencies for the test set T82-F for the exchange-correlation functional shown in each column. All quantities are in cm^{-1}.

		Expt.	Deviation = Theory - Experiment				
	Molecule		PBE	NCAPR	SCAN	PBE0	HSE06
1	H_2	4401.2	-85.8	-73.8	22.1	5.9	16.2
2	Li_2	351.4	-21.3	-26.6	-19.2	-12.9	-14.3
3	LiH	1405.7	-28.5	-37.1	-3.5	2.7	2.9
4	LiF	910.6	-16.4	-37.9	-5.1	6.4	1.4
5	LiCl	643.0	-3.6	-20.4	-7.0	7.7	5.5
6	LiO	814.6	-18.5	-35.3	-8.0	14.2	8.3
7	LiNa	256.8	-11.1	-17.3	-10.2	-4.5	-7.6
8	Be_2	267.9	78.7	55.1	60.6	27.1	28.9
9	BeH	2060.8	-86.3	-90.8	-31.7	-39.4	-38.5
10	BeH^+	2221.7	-112.5	-93.9	-25.5	-43.2	-41.0
11	BeF	1247.4	-41.2	-60.3	-10.6	-0.2	-5.3
12	BeCl	846.7	-32.7	-47.6	-24.7	-16.7	-21.5
13	BeO	1487.3	-33.2	-44.9	29.0	58.4	54.0
14	BeS	997.9	-20.4	-30.8	21.0	20.1	17.5
15	B_2	1051.3	-39.1	-58.6	-46.6	-31.2	-35.7
16	BH	2366.9	-124.4	-132.3	-47.6	-39.0	-41.8
17	BF	1402.1	-51.0	-73.2	-2.3	10.8	5.6
18	BCl	840.3	-31.0	-48.4	-3.7	0.0	-5.5
19	BN	1514.6	1.4	-20.3	61.2	89.5	82.1
20	BO	1885.7	-38.5	-56.7	16.6	50.7	45.7
21	BS	1180.2	-18.5	-32.5	28.4	27.5	22.3
22	C_2	1854.7	2.2	-20.9	44.6	46.7	41.8
23	CH	2858.5	-127.1	-144.3	-40.0	-16.7	-20.3
24	CF	1308.1	-54.2	-80.2	-3.8	42.0	34.8
25	CN	2068.6	25.3	3.3	86.1	116.6	110.9
26	CO	2169.8	-40.2	-59.9	41.6	70.0	64.9
27	CO^+	2214.2	-10.6	-33.6	78.6	121.9	115.8
28	CP	1239.7	9.6	-5.3	48.2	66.4	60.9
29	CS	1285.2	-22.9	-36.8	23.1	47.4	42.2
30	N_2	2358.6	-5.5	-24.0	75.9	125.1	120.7
31	N_2^+	2207.0	58.8	34.9	119.1	163.5	157.4
32	NH	3282.3	-109.1	-128.9	-26.8	24.8	20.2
33	NF	1141.4	-9.4	-36.0	23.4	81.4	72.3
34	NCl	828.0	8.8	-11.9	6.2	37.7	30.1
35	NO	1904.2	-11.8	-36.4	56.9	127.2	120.0
36	NO^+	2376.4	-13.7	-33.7	87.4	152.8	147.0
37	NS	1218.7	8.1	-22.0	43.2	73.9	67.5
38	O_2	1580.2	-21.9	-49.7	46.4	137.5	127.0
39	O_2^+	1904.8	32.3	3.2	122.7	228.9	219.5
40	OH	3737.8	-131.6	-155.2	-7.5	27.8	20.9
41	OH^+	3113.4	-157.5	-159.8	-40.4	-3.7	-3.1
42	F_2	916.6	78.2	59.0	125.6	180.7	170.2
43	F_2^+	1073.3	76.5	54.4	132.0	227.5	216.8
44	HF	4138.3	-158.6	-179.3	-35.1	21.0	17.2
45	HF^+	3090.5	-178.4	-178.8	-61.9	-27.4	-32.1
46	Na2	159.1	-0.7	-7.5	-0.2	3.2	-1.1
47	NaH	1172.2	-23.7	-38.8	13.8	8.3	1.7
48	NaF	535.7	-16.5	-28.3	7.3	3.7	0.5
49	NaO	492.3	-24.1	-31.7	0.8	2.5	-2.8
50	MgH	1495.2	-88.3	-89.1	-32.4	-31.6	-30.6
51	MgH^+	1699.1	-46.4	-43.3	20.6	18.7	14.9

Table S13 – continued

52	MgO	784.8	19.9	7.7	50.9	48.0	42.4
53	MgS	528.7	-1.6	-10.4	23.0	18.0	13.8
54	Al_2	350.0	-8.2	-19.2	1.1	-0.7	-3.2
55	AlH	1682.6	-100.2	-108.7	-41.8	-41.2	-40.3
56	AlF	802.3	-50.5	-61.4	-10.8	-14.1	-19.6
57	AlCl	481.3	-22.5	-31.9	-4.2	-6.4	-9.8
58	AlO	979.2	-19.1	-35.3	12.6	-3.7	-12.5
59	AlS	617.1	-15.7	-27.5	16.7	9.2	3.9
60	Si_2	511.0	-26.2	-34.0	51.9	58.0	53.3
61	SiH	2041.8	-92.8	-103.7	16.8	-24.9	-21.4
62	SiH^+	2157.2	-114.2	-114.6	-50.7	-37.8	-37.3
63	SiF	857.2	-45.4	-62.7	-11.8	-5.5	-10.4
64	SiCl	535.6	-13.0	-32.9	-11.6	-3.2	-8.9
65	SiN	1151.4	-1.6	-15.0	27.7	46.8	40.9
66	SiO	1241.5	-46.9	-56.4	11.3	30.9	26.2
67	SiS	749.6	-24.2	-32.7	7.8	16.8	10.8
68	P_2	780.8	1.4	-6.6	32.6	51.8	47.2
69	P_2^+	672.2	2.4	-5.9	108.5	126.7	121.7
70	PH	2365.2	-78.5	-92.0	23.3	3.2	4.7
71	PF	846.8	-37.9	-50.3	-0.1	16.0	5.8
72	PCl	551.4	-19.2	-24.8	-4.5	8.6	2.3
73	PN	1337.2	2.3	-9.3	54.7	91.4	86.2
74	PO	1233.3	-27.3	-48.4	22.2	52.0	46.8
75	S_2	725.6	-19.4	-34.3	10.6	30.6	24.9
76	SO	1149.2	-40.0	-57.3	15.0	51.7	45.1
77	Cl_2	559.7	-16.7	-31.9	-0.2	21.7	15.7
78	Cl_2^+	645.6	-20.6	-34.4	1.2	34.8	27.9
79	HCl	2990.9	-91.1	-107.8	-15.0	10.3	6.5
80	HCl+	2673.7	-113.4	-109.1	-37.1	-11.6	-7.6
81	ClF	786.1	-22.7	-40.0	4.6	42.2	34.6
82	ClO	853.8	9.5	-12.1	9.5	49.0	38.9

Table S14: Comparison of TDDFT valence and Rydberg excited states of small molecules with experimental values in eV.

Molecule		Exp.	PBE	NCAPR	PBE0	HSE06
N_2	V $^3\Pi_g$	8.04	7.41	7.54	7.53	7.52
	V $^3\Sigma_u^+$	7.75	7.55	7.74	6.97	6.95
	V $^3\Delta_u$	8.88	8.36	8.42	7.95	7.92
	V $^1\Pi_g$	9.31	9.10	9.13	9.32	9.32
	V $^3\Sigma_u^-$	9.67	9.69	9.71	9.37	9.37
	V $^1\Sigma_u^-$	9.92	9.69	9.71	9.37	9.37
	V $^1\Delta_u$	10.27	10.11	10.07	9.91	9.90
	R $^3\Sigma_g^+$	12.00	10.13	11.01	11.19	11.25
	R $^1\Sigma_g^+$	12.20	10.41	11.28	11.54	11.62
	V $^3\Pi_u$	11.19	10.43	10.63	10.79	10.79
CO	V $^3\Pi$	6.32	5.75	5.98	5.74	5.74
	V $^3\Sigma^+$	8.51	8.11	8.27	7.85	7.83
	V $^1\Pi$	8.51	8.25	8.30	8.43	8.44
	V $^3\Delta$	9.36	8.76	8.82	8.63	8.60
	R $^3\Sigma^+$	10.40	8.82	9.49	9.41	9.75
	R $^1\Sigma^+$	10.78	9.09	9.37	9.64	10.15
	R $^3\Sigma^+$	11.30	9.36	10.10	10.28	10.44
	R $^1\Sigma^+$	11.40	9.43	10.25	10.37	10.54
	R $^3\Pi$	11.55	9.44	9.51	9.82	10.54
	R $^1\Pi$	11.53	9.52	9.25	9.86	10.62
CH_2O	V $^3A_2$	3.50	3.06	3.17	3.14	3.15
	V $^1A_2$	3.94	3.80	3.86	3.93	3.94
	R $^3B_2$	6.83	5.56	6.23	6.44	6.46
	V $^3A_1$	5.53	5.81	5.94	5.29	5.27
	R $^1B_2$	7.09	5.72	6.32	6.64	6.67
	R $^3A_1$	7.79	6.29	6.91	7.27	7.32
	R $^1A_1$	7.97	6.36	6.92	7.37	7.44
	R $^3B_2$	7.96	6.39	7.09	7.26	7.32
	R $^1B_2$	8.12	6.46	7.12	7.37	7.44
	R $^1A_2$	8.38	6.63	7.70	7.60	7.71
C_2H_4	V $^3B_{1u}$	4.36	4.22	4.36	3.81	3.79
	R $^3B_{3u}$	6.98	6.25	6.93	6.66	6.68
	R $^1B_{3u}$	7.15	6.35	6.99	6.78	6.80
	R $^3B_{2g}$	7.79	6.73	7.54	7.24	7.26
	R $^1B_{2g}$	8.00	6.78	7.59	7.31	7.34
	R $^3B_{1g}$	7.79	6.76	7.19	7.24	7.27
	R $^1B_{1g}$	7.83	6.80	7.59	7.30	7.33
	R ^3A_g	8.15	7.00	7.62	7.47	7.53
	R ^1A_g	8.29	7.14	7.68	7.62	7.69
	V $^1B_{1u}$	7.66	7.24	7.44	7.44	7.44
	MAD		1.00	0.60	0.62	0.54

Table S15: Dipole moment in Debye.

System	CCSD(T)	PBE	NCAPR	SCAN	PBE0	HSE06
AlF	1.4729	1.3739	1.3231	1.2985	1.3962	1.3968
BF	0.8194	1.0485	1.0815	1.0579	0.9758	0.9722
BH2Cl	0.6838	0.4379	0.4467	0.5430	0.5896	0.5909
BH2F	0.8269	0.6182	0.5941	0.6813	0.7479	0.7474
BHCl2	0.6684	0.4815	0.4871	0.5578	0.5931	0.5938
BHF2	0.9578	0.7749	0.7532	0.8275	0.8890	0.8878
CH2BH	0.6238	0.5090	0.5186	0.5647	0.6294	0.6297
CH2BOH	2.2558	2.2669	2.2729	2.3136	2.2984	2.2955
CH3BH2	0.5751	0.7259	0.7135	0.6942	0.6636	0.6575
CH3BO	3.6779	3.6347	3.6222	3.7727	3.8219	3.8153
CH3Cl	1.8981	1.8196	1.8151	1.9208	1.8860	1.8810
CH3F	1.8083	1.6370	1.6211	1.7025	1.7356	1.7335
CH3Li	5.8304	5.4869	5.6199	5.7662	5.6978	5.7054
CH3NH2	1.3876	1.3181	1.3130	1.3502	1.3595	1.3553
CH3OH	1.7091	1.5951	1.5832	1.6496	1.6630	1.6594
CH3SH	1.5906	1.5730	1.5706	1.6312	1.6089	1.6029
ClCN	2.8496	2.9533	2.9477	3.0000	2.9868	2.9834
ClF	0.8802	0.7192	0.7034	0.7978	0.8227	0.8229
CO	0.1172	0.2239	0.2255	0.1273	0.1017	0.0991
CS	1.9692	2.0088	1.9917	1.9506	1.9418	1.9344
CSO	0.7327	0.7628	0.7361	0.8002	0.8059	0.8045
FCN	2.1756	2.3228	2.3370	2.3381	2.3037	2.3014
FNO	1.6971	1.4644	1.4598	1.5349	1.5940	1.5943
H2O	1.8601	1.7954	1.7834	1.8400	1.8578	1.8543
H2O-H2O	2.7303	2.7267	2.7150	2.7546	2.7620	2.7561
H2O-NH3	3.5004	3.5086	3.4845	3.5311	3.5492	3.5400
H2S-H2S	0.9181	1.0315	1.0119	1.0176	0.9987	0.9920
H2S-HCl	2.1328	2.2779	2.2484	2.3041	2.2531	2.2431
HBH2BH	0.8429	0.8614	0.8452	0.8446	0.8631	0.8545
HBO	2.7322	2.5855	2.5807	2.7311	2.7947	2.7929
HBS	1.3753	1.2268	1.2476	1.4045	1.4329	1.4322
HCCCl	0.5009	0.2646	0.2649	0.3306	0.3704	0.3679
HCCF	0.7452	0.4632	0.4440	0.5506	0.6128	0.6124
HCHO	2.3927	2.2376	2.2133	2.3641	2.3972	2.3925
HCl	1.1055	1.0681	1.0581	1.1249	1.1100	1.1054
HCl-HCl	1.7766	1.8196	1.8040	1.8691	1.8308	1.8231
HCN	3.0065	2.9427	2.9378	3.0341	3.0361	3.0333
HCNO	2.956	2.4233	2.4126	2.5996	2.7724	2.7650
HCOF	2.1169	1.9867	1.9825	2.0948	2.1207	2.1173
HCONH2	3.9152	3.8264	3.8323	3.9415	3.9656	3.9590
HCOOH	1.3835	1.4171	1.4345	1.4812	1.4661	1.4663
HF	1.8059	1.7455	1.7336	1.7851	1.8014	1.7987
HF-HF	3.3991	3.3552	3.3389	3.4064	3.4161	3.4111
HN3	1.6603	1.7542	1.7440	1.7479	1.6975	1.6945
HNC	3.0818	3.0654	3.0598	3.0530	3.0189	3.0112
HNCO	2.0639	1.9660	1.9510	2.0396	2.0467	2.0427
HOCl	1.5216	1.4974	1.4910	1.5321	1.5345	1.5318
HOCN	3.7998	3.8703	3.8959	3.9549	3.9329	3.9274
HOOH	1.5732	1.5239	1.5114	1.5533	1.5721	1.5694
LiBH4	6.1281	5.9476	6.0191	6.0738	6.0287	6.0347
LiCl	7.096	6.8442	6.9166	7.0322	6.9886	6.9915
LiCN	6.9851	6.8165	6.8970	6.9579	6.9238	6.9271
LiF	6.2879	6.0935	6.1406	6.2168	6.2175	6.2195

Table S15 – continued

LiH	5.8286	5.6155	5.7484	5.8493	5.7526	5.7578
LiOH	4.5664	4.3768	4.4527	4.5098	4.4863	4.4914
N2H4	2.7179	2.6368	2.6239	2.6693	2.7071	2.6988
NaCl	9.0066	8.4901	8.7068	8.8427	8.7842	8.7788
NaCN	8.8903	8.5643	8.7309	8.8039	8.7682	8.7688
NaF	8.1339	7.7239	7.8809	7.9817	7.9942	7.9927
NaH	6.3966	5.7562	6.0096	6.3337	6.2036	6.1851
NaOH	6.769	6.5523	6.6629	6.6753	6.6706	6.6774
NH2Cl	1.9468	1.9180	1.9158	2.0039	1.9683	1.9648
NH2F	2.2688	2.1472	2.1353	2.2572	2.2470	2.2436
NH2OH	0.7044	0.6306	0.6260	0.7007	0.6801	0.6794
NH3	1.5289	1.4748	1.4684	1.5090	1.5265	1.5225
NH3-BH3	5.281	5.2510	5.2653	5.3152	5.2903	5.2866
NH3-NH3	2.1345	2.1436	2.1312	2.1623	2.1679	2.1613
NH3O	5.3942	5.0477	5.0391	5.1806	5.2626	5.2491
OCl2	0.5625	0.4656	0.4565	0.4942	0.5349	0.5334
P2H4	0.9979	0.9672	0.9500	1.0243	1.0242	1.0110
PH2OH	0.6836	0.6610	0.6699	0.6432	0.6564	0.6648
PH3	0.6069	0.6025	0.5867	0.6429	0.6363	0.6249
PH3O	3.7704	3.4760	3.4578	3.6008	3.7147	3.7050
S2H2	1.1425	1.0913	1.0789	1.1485	1.1451	1.1367
SCl2	0.3891	0.2995	0.3005	0.3439	0.3512	0.3541
SF2	1.0555	0.7973	0.7780	0.8564	0.9557	0.9574
SH2	0.9939	0.9656	0.9531	1.0126	1.0095	1.0021
SiH3Cl	1.3645	1.2104	1.1977	1.2488	1.2927	1.2889
SiH3F	1.3123	1.1743	1.1410	1.2030	1.2667	1.2625
SiO	3.1123	2.9017	2.8843	3.0029	3.1502	3.1490
SO2	1.6286	1.4850	1.4767	1.5389	1.6228	1.6233
AlH2	0.4011	0.3481	0.3796	0.3992	0.3700	0.3795
BeH	0.2319	0.2434	0.2729	0.2866	0.2520	0.2610
BH2	0.5004	0.5102	0.5055	0.4699	0.5105	0.5054
BN	2.0366	1.8899	1.8866	2.1672	2.1858	2.1798
BO	2.3171	2.1837	2.1831	2.3566	2.4099	2.4092
BS	0.7834	0.6599	0.6767	0.8825	0.8704	0.8696
C2H	0.7601	0.7625	0.7712	0.7514	0.7534	0.7531
C2H3	0.6867	0.7214	0.7182	0.6786	0.6936	0.6884
C2H5	0.314	0.3808	0.3695	0.3319	0.3328	0.3276
CF	0.6793	0.9422	0.9515	0.8503	0.7848	0.7812
CF2	0.5402	0.7623	0.7789	0.7208	0.6447	0.6398
CH2F	1.3796	1.1533	1.1424	1.2648	1.3037	1.3038
CH2PH	0.8748	0.8990	0.9043	0.9951	0.9216	0.9162
CH2-t	0.5862	0.5896	0.5858	0.5636	0.5939	0.5908
CH3O	2.0368	2.1216	2.0908	2.0598	2.0418	2.0332
ClO2	1.8627	1.6696	1.6645	1.7237	1.7991	1.7988
CN	1.4318	1.1546	1.1276	1.4595	1.4833	1.4761
FCO	0.7678	0.7572	0.7613	0.8635	0.8586	0.8567
FH-BH2	2.973	3.0208	2.9756	2.9897	3.0472	3.0357
FH-NH2	4.6265	4.5641	4.5356	4.6489	4.6613	4.6507
FH-OH	3.3808	3.2676	3.2627	3.3917	3.4065	3.4000
H2CN	2.4939	2.4666	2.4537	2.5084	2.4886	2.4795
H2O-Al	4.3573	4.2175	4.3171	4.4480	4.3692	4.3647
H2O-Cl	2.2383	3.1191	3.1215	2.9277	2.6725	2.6708
H2O-F	2.1875	3.1722	3.1486	2.8458	2.6744	2.6715
H2O-Li	3.6184	2.3975	2.4497	2.7992	3.1284	3.0805
HCHS	1.7588	1.6712	1.6847	1.8378	1.7733	1.7699
HCO	1.6912	1.5537	1.5438	1.6793	1.7201	1.7160

Table S15 – continued

HCP	0.3542	0.3710	0.3845	0.4530	0.3599	0.3589
HNO	1.6536	1.4845	1.4635	1.5600	1.6347	1.6263
HNO2	1.9345	1.8829	1.8750	1.9506	1.9599	1.9531
HNS	1.4062	1.3359	1.3285	1.3686	1.3820	1.3780
HO2	2.1659	2.2112	2.1967	2.1340	2.1567	2.1497
HPO	2.6291	2.2390	2.2216	2.3434	2.4608	2.4567
LiN	7.0558	6.5489	6.7078	6.8840	6.9185	6.9167
N2H2	2.8771	2.7650	2.7468	2.8025	2.8553	2.8448
NCl	1.1279	1.2727	1.2641	1.1267	1.1154	1.1124
NCO	0.7935	0.8619	0.8639	0.8641	0.7935	0.7928
NF	0.0671	0.3136	0.3198	0.1586	0.1175	0.1148
NF2	0.1904	0.0318	0.0288	0.1429	0.1711	0.1741
NH	1.5433	1.4815	1.4670	1.5281	1.5316	1.5270
NH2	1.7853	1.7201	1.7107	1.7644	1.7778	1.7725
NO	0.1271	0.2292	0.2287	0.1199	0.1121	0.1102
NO2	0.335	0.2753	0.2646	0.3100	0.3542	0.3540
NOCl	2.0773	1.7388	1.7727	1.8447	1.8860	1.8826
NP	2.8713	2.7212	2.7065	2.7648	2.8819	2.8756
NS	1.8237	1.7674	1.7508	1.7200	1.7827	1.7825
OCl	1.279	1.3439	1.3259	1.2061	1.2447	1.2410
OF	0.0205	0.1938	0.1905	0.0324	0.0179	0.0202
OF2	0.3252	0.2795	0.2799	0.3254	0.3261	0.3279
OH	1.655	1.5940	1.5831	1.6412	1.6480	1.6446
PCl	0.5657	0.3086	0.2954	0.4024	0.4747	0.4771
PF	0.8104	0.5715	0.5447	0.6164	0.7203	0.7218
PH	0.4375	0.4202	0.4108	0.4750	0.4552	0.4488
PH2	0.5472	0.5357	0.5213	0.5891	0.5731	0.5631
PO	1.9617	1.7658	1.7480	1.8685	1.9947	1.9918
PO2	1.4426	1.2608	1.2414	1.3785	1.4372	1.4362
PPO	1.8812	1.6797	1.6525	1.7665	1.8732	1.8699
PS	0.6825	0.4938	0.4915	0.6027	0.6467	0.6441
SCl	0.069	0.1797	0.1845	0.0468	0.0089	0.0104
SF	0.8139	0.5423	0.5220	0.6300	0.7258	0.7272
SH	0.7727	0.7449	0.7358	0.7960	0.7825	0.7767
SO-trip	1.5606	1.3581	1.3383	1.3927	1.5086	1.5078
MAD		0.1529	0.1451	0.0892	0.0626	0.0618

Table S16: Static and dynamic polarizabilities in a.u.

System	Freq a.u.	Reff	LDA	PBE	CAP	NCAPR
		MC-SCF				
H_2O	0.00	9.210	10.12	10.14	9.46	9.71
	0.05	9.284	10.22	10.25	9.55	9.80
	0.10	9.520	10.58	10.62	9.85	10.12
	0.15	9.960	11.33	11.41	10.45	10.77
	0.20	10.770	13.07	13.36	11.73	12.16
	0.25	12.560	174.40	-8.91	19.38	22.15
NH_3	0.00	13.880	14.83	14.75	13.80	14.15
	0.05	14.047	15.05	14.97	13.97	14.34
	0.10	14.600	15.80	15.74	14.57	14.98
	0.15	15.784	17.65	17.71	15.95	16.47
	0.20	18.840	29.24	34.42	21.04	22.22
CH_4	0.00	15.616	17.49	17.22	16.35	16.55
	0.05	15.740	17.66	17.39	16.49	16.70
	0.10	16.129	18.20	17.92	16.95	17.17
	0.15	16.836	19.22	18.93	17.80	18.05
	0.20	17.976	20.96	20.65	19.23	19.51
	0.25	19.798	24.12	23.82	21.71	22.04
	0.30	22.933	31.96	31.96	27.14	27.47
HF	0.00	5.324	5.89	5.94	5.56	5.68
	0.10	5.429	6.05	6.12	5.70	5.83
	0.20	5.795	6.68	6.79	6.23	6.38
	0.30	6.692	9.26	9.98	8.09	8.34
	0.40	17.012	6.68	7.09	5.50	5.63
H_2	0.00	5.203	5.56	5.34	5.20	5.24
	0.10	5.392	5.78	5.55	5.39	5.44
	0.20	6.061	6.59	6.31	6.08	6.15
	0.30	7.740	8.67	8.24	7.80	7.91
		CCSD				
N_2	0.0000	11.60	11.81	11.76	11.28	11.49
	0.0720	11.75	11.99	11.94	11.44	11.66
	0.0886	11.83	12.08	12.03	11.52	11.74
	0.0934	11.84	12.11	12.06	11.55	11.77
	0.0995	11.89	12.15	12.10	11.59	11.81
CO	0.0000	13.07	13.40	13.36	12.72	12.92
	0.0720	13.32	13.70	13.66	12.98	13.19
	0.0886	13.46	13.86	13.81	13.12	13.33
	0.0934	13.5	13.91	13.87	13.16	13.38
	0.0995	13.57	13.99	13.94	13.23	13.45
CO_2	0.0000	18.00	17.44	17.51	16.71	17.00
	0.0720	18.27	17.70	17.78	16.95	17.25
	0.0886	18.42	17.85	17.93	17.08	17.39
	0.0934	18.46	17.89	17.98	17.13	17.43
	0.0995	18.53	17.96	18.04	17.18	17.49
Cl_2	0.0000	30.86	30.37	30.04	28.73	29.45
	0.0720	31.52	31.08	30.75	29.34	30.11
	0.0886	31.89	31.50	31.15	29.69	30.48
	0.0934	32.01	31.64	31.29	29.81	30.61
	0.0995	32.18	31.86	31.50	29.97	30.79
C_2H_2	0.0000	22.25	23.38	23.29	21.94	22.52
	0.0720	22.82	24.07	24.00	22.53	23.15

Table S16 – continued

	0.0886	23.14	24.44	24.38	22.85	23.49
	0.0934	23.24	24.57	24.51	22.96	23.61
	0.0995	23.38	24.74	24.69	23.10	23.77
OCS	0.0000	35.71	34.08	34.01	32.37	33.15
	0.0720	36.80	35.11	35.04	33.27	34.10
	0.0886	37.36	35.67	35.60	33.77	34.63
	0.0934	37.57	35.86	35.79	33.93	34.80
	0.0995	37.88	36.12	36.05	34.16	35.05
CS_2	0.0000	59.15	54.40	54.25	51.56	52.85
	0.0720	62.04	56.89	56.74	53.79	55.19
	0.0886	63.77	58.31	58.16	55.05	56.52
	0.0934	64.40	58.80	58.65	55.49	56.97
	0.0995	65.20	59.48	59.33	56.09	57.61
MAD			4.44	2.25	1.92	1.77

Table S17: Electron affinities in eV. Theoretical values determined through energy differences.

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06
1,1-Dichloroethylene	-0.75[a]	-1.365	-0.379	-0.961	-0.460	-1.017
1,3-Cyclohexadiene	-0.80[a]	-0.820	-0.437	-0.471	-0.559	-0.692
Acetaldehyde	-1.19[a]	-0.369	-0.362	-0.474	-0.411	-0.400
Adenine	-0.64[a]	-0.520	-0.106	-0.696	-0.209	-0.785
Bromobenzene	-0.70[a]	-0.878	-0.870	-0.832	-0.939	-0.942
Chlorobenzene	-0.75[a]	-0.931	-0.925	-0.885	-0.365	-0.995
Chloroethylene	-1.29[a]	-2.429	-0.442	-0.556	-0.491	-0.478
Chloromethane	-3.45[a]	-0.374	-0.360	-0.473	-0.426	-0.418
cis-Dichloroethylene	-1.12[a]	-0.346	-0.361	-0.461	-0.401	-0.392
Cytosine	-0.36[a]	-0.594	-0.576	-0.582	-0.619	-0.620
Ethylene	-1.78[a]	-3.214	-0.503	-0.635	-0.569	-3.338
Fluorobenzene	-0.87[a]	-1.074	-0.360	-1.036	-0.492	-1.122
Naphthalene	-0.20[a]	-0.207	-0.206	-0.164	-0.298	-0.299
Norbornadiene	-1.04[a]	-1.075	-0.364	-0.531	-0.513	-0.634
Pyrazine	-0.07[a]	-0.200	-0.200	-0.158	-0.220	-0.224
Pyridazine	-0.32[a]	-0.268	-0.263	-0.203	-0.282	-0.285
Pyrimidine	-0.25[a]	-0.446	-0.269	-0.397	-0.491	-0.493
Styrene	-0.25[a]	-0.257	-0.255	-0.249	-0.362	-0.359
Thiophene	-1.17[a]	-1.220	-1.184	-1.224	-0.548	-1.254
trans-Dichloroethylene	-0.82[a]	-0.975	-0.950	-0.970	-1.009	-1.009
Trichloroethylene	-0.58[a]	-0.570	-0.383	-0.702	-0.479	-0.769
Uracil	-0.21[a]	-0.447	-0.419	-0.286	-0.337	-0.480
1,2,4-Trimethylbenzene	-1.07[a]	-0.641	-0.351	-0.463	-0.410	-1.432
Acetone	-1.51[a]	-0.285	-0.301	-0.399	-0.348	-0.333
Aniline	-1.13[a]	-1.396	-0.382	-0.633	-0.507	-1.179
Anisole	-1.09[a]	-1.078	-0.307	-1.287	-0.431	-1.371
cis-Butene	-2.22[a]	-0.391	-0.419	-0.527	-0.474	-0.448
Cyclohexene	-2.07[a]	-0.338	-0.381	-0.482	-0.435	-0.404
Furan	-1.76[a]	-2.262	-0.421	-0.535	-0.475	-0.451
m-Xylene	-1.06[a]	-1.304	0.000	-0.462	-0.493	-1.419
o-Xylene	-1.12[a]	-1.443	-1.403	-1.446	-0.420	-1.539
Phenol	-1.01[a]	-1.243	-1.224	-0.579	-1.311	-1.311
Propene	-1.99[a]	-0.657	-0.457	-0.577	-0.516	-0.496
Pyrrole	-2.38[a]	-0.891	-0.292	-0.761	-0.351	-0.339
trans-Butene	-2.10[a]	-0.545	-0.448	-0.627	-0.577	-0.584
Trimethylethylene	-2.24[a]	-0.493	-0.399	-0.498	-0.447	-0.417
CO2	-3.80[a]	-0.760	-0.742	-0.864	-0.837	-0.833
Guanine	-0.46[a]	0.121	0.037	-0.076	0.005	0.045
HC	1.24[b]	1.520	1.526	1.478	1.379	1.371
H3C	0.08[b]	0.030	0.095	-0.271	-0.197	-0.206
H2N	0.77[b]	0.821	0.872	0.462	0.545	0.539
HO	1.83[b]	1.951	1.991	1.602	1.594	1.592
HSi	1.28[b]	1.385	1.413	1.454	1.361	1.353
H2Si	1.12[b]	1.248	1.282	1.365	1.229	1.223
H3Si	1.41[b]	0.945	1.006	0.826	0.855	0.848
H2P	1.27[b]	1.237	1.296	1.125	1.154	1.144
HS	2.36[b]	2.327	2.383	2.224	2.236	2.228
NO	0.02[b]	-0.101	-0.079	-0.070	-0.088	-0.085
CN	3.86[b]	3.757	3.823	3.809	3.905	3.900
OP	1.09[b]	1.163	1.190	1.301	1.242	1.241
Cl2	2.39[b]	1.235	1.265	1.351	1.260	1.260
C2	3.27[b]	3.547	3.574	4.309	4.358	4.352
CF2	0.18[b]	-0.099	-0.086	-0.010	-0.078	-0.076

Table S17 – continued

CNO	3.61[b]	3.359	3.369	3.267	3.337	3.327
NO2	2.27[b]	1.266	1.272	1.197	1.382	1.381
O3	2.10[b]	1.777	1.781	2.051	2.252	2.249
OF	2.27[b]	1.773	1.796	1.627	1.742	1.742
O2S	1.11[b]	1.004	1.020	1.192	1.249	1.249
OS2	1.88[b]	1.763	1.793	1.974	2.048	2.043
HC2	2.97[b]	2.948	3.013	2.867	2.919	2.915
H3C2	0.67[b]	0.247	0.319	-0.003	0.066	0.066
H3C3	0.89[b]	0.719	0.742	0.456	0.608	0.599
H5C3	0.47[b]	0.452	0.472	0.123	0.288	0.280
HCO	0.31[b]	-0.026	0.084	-0.136	-0.139	-0.129
HCF	0.54[b]	0.505	0.523	0.591	0.466	0.465
CH3O	1.57[b]	1.411	1.448	1.124	1.189	1.191
H3CS	1.87[b]	-0.203	-0.162	-0.436	-0.339	-0.344
H2CS	0.47[b]	0.433	0.464	0.564	0.492	0.491
CH2CHO	1.82[b]	1.738	1.744	1.517	1.584	1.575
CH3CO	0.42[b]	0.291	0.308	0.089	0.041	0.053
H5C2O	1.71[b]	1.646	1.640	1.335	1.370	1.369
HLi	0.34[b]	0.434	0.475	0.364	0.423	0.422
HNO	0.34[b]	0.291	0.242	0.325	0.226	0.232
HO2	1.08[b]	0.486	0.494	0.333	0.400	0.403
CS	0.21[c]	0.089	0.134	0.181	0.150	0.152
ClO	2.28[c]	2.003	2.037	1.892	2.022	2.019
Na2	0.43[c]	0.453	0.516	0.493	0.450	0.448
P2	0.59[c]	0.581	0.631	0.659	0.666	0.664
COS	0.46[c]	-0.768	-0.740	-0.899	-0.856	-0.846
CS2	0.90[c]	0.003	0.040	0.091	0.133	0.131
N2O	0.22[c]	-1.170	-1.141	-1.313	-1.285	-1.270
NH2 rad	0.77[c]	0.821	0.872	0.463	0.545	0.539
CH3NO2	0.48[c]	0.044	0.024	0.006	-0.098	-0.047
MAD		0.488	0.542	0.550	0.581	0.553

[a] D. Zhang, X. Yang, X. Zheng and W. Yang, Molecular Physics **116** 927 (2018). [b] X. Zheng, A. J. Cohen, P. Mori-Sanchez, X. Hu and W. Yang, Phys. Rev. Lett. **107** 026403 (2011). [c] R. G. Parr, L. v. Szentpály and S. Liu , J. Am. Chem. Soc. **121** 1922 (1999).

Table S18: Ionization potentials in eV. Theoretical values determined through energy differences.

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06
1,1-Dichloroethylene	10.00[a]	9.636	9.650	9.664	9.811	9.798
1,3-Cyclohexadiene	8.32[a]	8.043	8.053	7.942	8.078	8.068
Acetaldehyde	10.24[a]	10.004	10.038	9.930	10.077	10.080
Adenine	8.44[b]	8.132	8.132	8.124	8.253	8.238
Bromobenzene	9.00[a]	12.516	12.516	8.767	8.939	8.917
Chlorobenzene	9.07[a]	8.924	8.932	8.896	9.058	9.040
Chloroethylene	10.20[a]	9.901	9.915	9.889	9.986	9.976
Chloromethane	11.29[a]	11.130	11.176	11.186	11.251	11.251
cis-Dichloroethylene	9.80[a]	9.458	9.477	9.530	9.661	9.651
Cytosine	8.80[c]	8.563	8.566	8.519	8.682	8.666
Ethylene	10.68[a]	10.665	10.653	10.466	10.492	10.481
Fluorobenzene	9.22[a]	9.149	9.146	9.088	9.229	9.215
Naphthalene	8.14[a]	7.913	7.912	7.790	7.981	7.961
Norbornadiene	8.38[a]	8.353	8.355	8.247	8.435	8.417
Pyrazine	9.63[a]	9.030	9.074	9.197	9.513	9.501
Pyridazine	9.31[a]	8.795	8.841	8.911	9.078	9.075
Pyrimidine	9.73[a]	9.205	9.242	9.302	9.597	9.584
Styrene	8.48[a]	8.259	8.257	8.118	8.303	8.283
Thiophene	8.86[a]	8.924	8.922	8.766	8.904	8.889
trans-Dichloroethylene	9.80[a]	9.415	9.436	9.500	9.635	9.623
Trichloroethylene	9.60[a]	9.226	9.246	9.328	9.486	9.473
Uracil	9.68[a]	9.283	9.284	9.292	9.434	9.418
1,2,4-Trimethylbenzene	8.50[a]	8.132	8.143	8.030	8.198	8.185
Acetone	9.80[a]	9.460	9.482	9.396	9.553	9.551
Aniline	7.72[a]	7.758	7.769	7.668	7.824	7.812
Anisole	8.20[a]	8.113	8.119	8.047	8.226	8.211
cis-Butene	9.32[a]	9.039	9.059	8.953	9.060	9.053
Cyclohexene	9.09[a]	8.847	8.870	8.788	8.897	8.890
Furan	8.90[a]	8.917	8.911	8.781	8.864	8.851
m-Xylene	8.55[a]	8.470	8.478	8.340	8.518	8.503
o-Xylene	8.56[d]	8.476	8.483	8.356	8.519	8.505
Phenol	8.75[a]	8.409	8.413	8.341	8.493	8.479
Propene	9.91[a]	9.747	9.757	9.619	9.703	9.694
Pyrrole	8.23[a]	8.299	8.296	8.126	8.236	8.223
trans-Butene	9.37[a]	9.025	9.047	8.960	9.053	9.046
Trimethylethylene	8.69[a]	8.576	8.597	8.504	8.608	8.602
CO2	13.78[a]	13.668	13.668	13.592	13.748	13.741
Guanine	8.24[e]	7.834	7.832	7.804	7.955	7.939
HC	10.23[f]	11.021	11.024	11.156	10.993	11.005
H3C	9.84[g]	10.014	10.004	10.106	9.957	9.960
H2N	11.14[g]	12.212	12.296	12.006	12.067	12.085
HO	13.01[g]	13.264	13.322	13.151	13.065	13.081
HSi	7.89[a]	8.053	8.092	8.207	8.080	8.084
H2Si	9.15[g]	9.362	9.447	9.321	9.363	9.372
H3Si	8.14[g]	8.930	8.969	9.093	8.976	8.982
H2P	9.82[g]	9.978	10.001	10.180	10.015	10.018
HS	10.37[g]	10.394	10.473	10.388	10.363	10.369
NO	9.26[f]	9.977	9.987	10.224	10.275	10.286
CN	13.60[g]	14.248	14.255	14.036	14.047	14.046
OP	8.39[a]	8.587	8.616	8.800	8.788	8.795
Cl2	11.50[g]	11.290	11.331	11.491	11.569	11.565
C2	11.40[f]	12.936	12.960	12.323	12.368	12.365
CF2	11.42[g]	11.898	11.944	11.964	12.122	12.128

Table S18 – continued

CNO	11.76[a]	12.014	12.035	12.040	12.039	12.039
NO2	9.59[f]	11.257	11.258	11.596	11.783	11.785
O3	12.73[a]	12.535	12.547	12.650	13.009	13.006
OF	12.78[f]	12.796	12.843	12.859	13.102	13.116
O2S	12.35[f]	12.064	12.082	12.178	12.356	12.350
OS2	10.58[a]	10.415	10.441	10.441	10.503	10.496
HC2	11.61[f]	11.617	11.633	11.408	11.455	11.454
H3C2	8.25[a]	9.568	9.598	9.773	9.723	9.733
H3C3	8.67[a]	8.648	8.652	8.822	8.768	8.764
H5C3	8.18[a]	8.110	8.115	8.331	8.184	8.181
HCO	8.14[g]	9.549	9.582	9.762	9.775	9.790
HCF	10.06[a]	10.371	10.442	10.382	10.493	10.508
CH3O	10.73[g]	10.553	10.626	10.601	10.707	10.723
H3CS	9.26[a]	7.777	7.801	7.993	7.952	7.955
H2CS	9.38[g]	9.264	9.313	9.182	9.269	9.268
CH2CHO	10.85[a]	10.109	10.143	10.029	10.117	10.120
CH3CO	7.00[a]	8.476	8.488	8.682	8.717	8.725
H5C2O	9.11[a]	9.985	10.051	10.123	10.221	10.233
HLi	7.90[a]	8.012	8.223	7.928	7.963	7.996
HNO	10.10[f]	10.349	10.402	10.380	10.513	10.526
HO2	11.35[f]	11.434	11.485	11.459	11.553	11.564
CS	11.33[f]	11.320	11.394	11.329	11.405	11.410
ClO	10.95[f]	10.820	10.870	10.887	11.077	11.083
Na2	4.98[f]	5.180	5.119	4.897	5.059	5.076
P2	10.53[f]	10.523	10.551	10.721	10.765	10.758
COS	11.18[f]	11.230	11.251	11.226	11.272	11.266
CS2	10.07[f]	10.043	10.075	10.027	10.072	10.068
N2O	12.89[f]	12.901	12.898	12.776	12.826	12.823
NH2 rad	11.14[f]	12.226	12.310	12.020	12.082	12.100
CH3NO2	11.08[f]	11.047	11.070	11.179	11.356	11.350
MAD		0.390	0.395	0.381	0.324	0.330

[a] http://webbook.nist.gov. [b] J. Lin, C. Yu, S. Peng, I. Akiyama, K. Li, L. K. Lee, P. R. Lebreton, J. Am. Chem. Soc. **102** 4627 (1980). [c] S. Urano, X. Yang, P. R. LeBreton, J. Mol. Struct. **214** 315 (1898). [d] http://goodforgas.com/wp-content/uploads/2013/12/TN2004_PID_gas_table_01_16_09.pdf. [e] J. Lin, C. Yu, S. Peng, I. Akiyama, K. Li, L. Lee, P. R. LeBreton, J. Phys. Chem. **84** 1006 (1980). [f] R. G. Parr, L. v. Szentpály and S. Liu , J. Am. Chem. Soc. **121** 1922 (1999). [g] X. Zheng, A. J. Cohen, P. Mori-Sanchez, X. Hu and W. Yang, Phys. Rev. Lett. **107** 026403 (2011).

Table S19: Band gaps in eV. Theoretical values determined through energy differences.

System	Exp.[a]	PBE	NCAPR	SCAN	PBE0	HSE06
1,1-Dichloroethylene	10.75	11.001	10.028	10.624	10.271	10.815
1,3-Cyclohexadiene	9.12	8.863	8.489	8.413	8.637	8.760
Acetaldehyde	11.43	10.374	10.400	10.403	10.488	10.480
Adenine	9.08	8.652	8.238	8.820	8.462	9.023
Bromobenzene	9.70	13.394	13.386	9.599	9.878	9.859
Chlorobenzene	9.82	9.855	9.856	9.781	9.423	10.035
Chloroethylene	11.49	12.330	10.357	10.445	10.477	10.454
Chloromethane	14.74	11.504	11.536	11.659	11.677	11.669
cis-Dichloroethylene	10.92	9.804	9.838	9.992	10.062	10.043
Cytosine	9.16	9.157	9.142	9.101	9.302	9.287
Ethylene	12.46	13.879	11.156	11.101	11.061	13.819
Fluorobenzene	10.09	10.224	9.506	10.124	9.722	10.337
Naphthalene	8.34	8.120	8.117	7.954	8.279	8.260
Norbornadiene	9.42	9.428	8.718	8.779	8.948	9.051
Pyrazine	9.70	9.230	9.273	9.355	9.734	9.725
Pyridazine	9.63	9.064	9.103	9.114	9.360	9.361
Pyrimidine	9.98	9.651	9.511	9.699	10.088	10.077
Styrene	8.73	8.515	8.513	8.367	8.665	8.642
Thiophene	10.03	10.144	10.106	9.990	9.452	10.143
trans-Dichloroethylene	10.62	10.390	10.386	10.470	10.643	10.631
Trichloroethylene	10.18	9.796	9.629	10.030	9.965	10.243
Uracil	9.89	9.730	9.703	9.578	9.771	9.899
1,2,4-Trimethylbenzene	9.57	8.773	8.494	8.494	8.608	9.617
Acetone	11.31	9.745	9.783	9.795	9.902	9.884
Aniline	8.85	9.154	8.151	8.300	8.331	8.990
Anisole	9.29	9.191	8.426	9.335	8.657	9.582
cis-Butene	11.54	9.429	9.479	9.481	9.534	9.500
Cyclohexene	11.16	9.186	9.251	9.270	9.332	9.293
Furan	10.66	11.179	9.332	9.316	9.339	9.302
m-Xylene	9.61	9.774	8.478	8.802	9.011	9.922
o-Xylene	9.68	9.919	9.886	9.802	8.940	10.044
Phenol	9.76	9.652	9.637	8.920	9.804	9.790
Propene	11.90	10.404	10.214	10.196	10.219	10.190
Pyrrole	10.61	9.190	8.588	8.887	8.587	8.562
trans-Butene	11.47	9.570	9.495	9.587	9.630	9.630
Trimethylethylene	10.93	9.068	8.996	9.001	9.055	9.019
CO2	17.58	14.428	14.410	14.456	14.584	14.574
Guanine	8.70	7.713	7.795	7.880	7.950	7.894
HC	8.99	9.501	9.498	9.678	9.614	9.635
H3C	9.76	9.984	9.909	10.377	10.154	10.165
H2N	10.37	11.391	11.424	11.543	11.522	11.546
HO	11.18	11.313	11.331	11.549	11.470	11.490
HSi	6.61	6.668	6.679	6.753	6.718	6.732
H2Si	8.03	8.114	8.165	7.956	8.134	8.149
H3Si	6.73	7.985	7.963	8.267	8.121	8.134
H2P	8.55	8.740	8.705	9.056	8.861	8.873
HS	8.01	8.067	8.090	8.164	8.128	8.141
NO	9.24	10.078	10.065	10.294	10.363	10.371
CN	9.74	10.491	10.431	10.226	10.142	10.146
OP	7.30	7.424	7.426	7.499	7.546	7.554
Cl2	9.11	10.055	10.066	10.139	10.309	10.304
C2	8.13	9.389	9.387	8.014	8.009	8.013
CF2	11.24	11.997	12.029	11.975	12.199	12.204

Table S19 – continued

CNO	8.15	8.655	8.666	8.773	8.702	8.711
NO2	7.32	9.991	9.985	10.399	10.401	10.404
O3	10.63	10.758	10.766	10.598	10.757	10.757
OF	10.51	11.023	11.047	11.232	11.360	11.373
O2S	11.24	11.060	11.062	10.987	11.107	11.101
OS2	8.70	8.651	8.648	8.467	8.455	8.453
HC2	8.64	8.669	8.620	8.542	8.537	8.539
H3C2	7.58	9.321	9.280	9.776	9.657	9.667
H3C3	7.78	7.928	7.910	8.366	8.160	8.165
H5C3	7.71	7.658	7.643	8.208	7.896	7.901
HCO	7.83	9.574	9.498	9.898	9.914	9.919
HCF	9.52	9.866	9.919	9.792	10.027	10.043
CH3O	9.16	9.142	9.178	9.477	9.517	9.531
H3CS	7.39	7.980	7.963	8.429	8.291	8.298
H2CS	8.91	8.831	8.849	8.619	8.777	8.777
CH2CHO	9.03	8.371	8.399	8.512	8.533	8.545
CH3CO	6.58	8.185	8.180	8.594	8.676	8.672
H5C2O	7.40	8.339	8.412	8.788	8.851	8.864
HLi	7.56	7.578	7.748	7.564	7.540	7.574
HNO	9.76	10.058	10.160	10.055	10.287	10.294
HO2	10.27	10.948	10.991	11.126	11.153	11.161
CS	11.12	11.231	11.260	11.148	11.255	11.258
ClO	8.67	8.817	8.833	8.995	9.055	9.064
Na2	4.55	4.727	4.603	4.404	4.609	4.628
P2	9.94	9.942	9.920	10.062	10.099	10.093
COS	10.72	11.998	11.991	12.126	12.128	12.112
CS2	9.17	10.041	10.035	9.936	9.939	9.936
N2O	12.67	14.070	14.039	14.089	14.111	14.092
NH2 rad	10.37	11.405	11.438	11.557	11.537	11.561
CH3NO2	10.60	11.002	11.045	11.173	11.454	11.398
MAD		0.729	0.811	0.791	0.786	0.737

[a] Values from Table S17 and Table S18.

Table S20: Electron affinities in eV. Theoretical values determined through the negative of the LUMO.

System	Exp.[a]	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[b]
1,1-Dichloroethylene	-0.75	1.721	1.693	1.501	0.789	1.162	-0.788
1,3-Cyclohexadiene	-0.80	1.722	1.711	1.505	0.783	1.157	-0.436
Acetaldehyde	-1.19	2.019	1.997	1.691	0.807	1.198	-0.348
Adenine	-0.64	1.654	1.635	1.443	0.763	1.127	-0.596
Bromobenzene	-0.70	1.607	1.595	1.419	0.711	1.079	-0.786
Chlorobenzene	-0.75	1.587	1.573	1.401	0.690	1.059	-0.826
Chloroethylene	-1.29	1.423	1.394	1.161	0.444	0.820	-1.079
Chloromethane	-3.45	0.905	0.674	0.378	0.221	0.517	-1.942
cis-Dichloroethylene	-1.12	1.588	1.582	1.400	0.633	1.010	-0.857
Cytosine	-0.36	1.987	1.976	1.826	1.110	1.483	-0.305
Ethylene	-1.78	1.069	1.032	0.717	0.058	0.434	-1.504
Fluorobenzene	-0.87	1.518	1.501	1.329	0.632	1.003	-0.902
Naphthalene	-0.20	2.074	2.068	1.921	1.252	1.611	-0.158
Norbornadiene	-1.04	1.380	1.338	1.155	0.424	0.792	-0.873
Pyrazine	-0.07	2.623	2.614	2.486	1.663	2.040	0.289
Pyridazine	-0.32	2.575	2.567	2.412	1.617	1.994	0.368
Pyrimidine	-0.25	2.373	2.361	2.174	1.398	1.775	0.014
Styrene	-0.25	2.046	2.031	1.863	1.194	1.556	-0.248
Thiophene	-1.17	1.385	1.388	1.234	0.520	0.894	-0.939
trans-Dichloroethylene	-0.82	1.740	1.718	1.556	0.794	1.170	-0.717
Trichloroethylene	-0.58	1.883	1.874	1.731	0.975	1.349	-0.560
Uracil	-0.21	2.380	2.366	2.222	1.480	1.854	-0.052
1,2,4-Trimethylbenzene	-1.07	0.993	0.955	0.781	0.134	0.493	-1.295
Acetone	-1.51	1.647	1.626	1.316	0.487	0.870	-0.648
Aniline	-1.13	1.061	1.042	0.865	0.187	0.555	-1.054
Anisole	-1.09	1.166	1.150	0.975	0.283	0.651	-1.052
cis-Butene	-2.22	0.363	0.349	0.042	-0.652	-0.279	-1.961
Cyclohexene	-2.07	0.632	0.431	0.185	-0.601	-0.109	-1.866
Furan	-1.76	0.857	0.830	0.669	-0.066	0.308	-1.444
m-Xylene	-1.06	1.099	1.070	0.881	0.224	0.587	-1.237
o-Xylene	-1.12	1.006	0.979	0.789	0.124	0.487	-1.329
Phenol	-1.01	1.264	1.247	1.074	0.385	0.754	-0.994
Propene	-1.99	0.744	0.704	0.405	-0.230	0.135	-1.714
Pyrrole	-2.38	0.122	0.092	-0.096	-0.751	-0.393	-2.050
trans-Butene	-2.10	0.442	0.402	0.115	-0.536	-0.170	-1.908
Trimethylethylene	-2.24	0.487	0.427	0.157	-0.368	-0.042	-1.812
CO2	-3.80	0.301	0.271	-0.133	-0.897	-0.515	-2.758
Guanine	-0.46	1.366	1.325	1.128	0.402	0.756	-0.848
HC	1.24	5.369	5.288	4.844	3.875	4.259	2.945
H3C	0.08	2.944	2.859	2.142	1.627	2.000	0.650
H2N	0.77	4.531	4.476	3.566	2.823	3.212	1.811
HO	1.83	6.444	6.389	5.405	4.297	4.694	3.705
HSi	1.28	4.239	4.230	4.028	3.304	3.672	2.250
H2Si	1.12	4.062	4.050	3.878	3.142	3.513	1.715
H3Si	1.41	3.548	3.510	3.057	2.594	2.963	1.309
H2P	1.27	4.209	4.221	3.715	3.122	3.495	1.853
HS	2.36	5.794	5.817	5.281	4.513	4.895	3.394
NO	0.02	4.315	4.291	4.003	2.885	3.288	2.298
CN	3.86	7.672	7.731	7.148	6.421	6.817	4.639
OP	1.09	4.489	4.493	4.367	3.531	3.917	2.477
Cl2	2.39	4.667	4.677	4.589	3.599	3.986	1.987
C2	3.27	7.143	7.156	8.044	7.035	7.428	4.334
CF2	0.18	3.740	3.698	3.553	2.498	2.894	1.025

Table S20 – continued

CNO	3.61	7.269	7.254	6.817	5.903	6.286	4.510
NO2	2.27	5.162	5.160	4.833	4.015	4.414	2.669
O3	2.10	6.094	6.091	6.164	5.159	5.558	3.301
OF	2.27	6.564	6.556	5.835	4.767	5.167	3.926
O2S	1.11	4.676	4.683	4.679	3.784	4.177	1.867
OS2	1.88	4.977	5.002	5.039	4.259	4.640	2.423
HC2	2.97	6.370	6.337	5.701	4.951	5.351	3.656
H3C2	0.67	3.159	3.152	2.388	1.877	2.257	0.910
H3C3	0.89	3.620	3.606	3.022	2.477	2.844	1.467
H5C3	0.47	3.247	3.228	2.530	2.061	2.427	1.197
HCO	0.31	3.305	3.361	2.827	2.092	2.494	1.255
HCF	0.54	4.241	4.191	3.977	2.916	3.308	1.860
CH3O	1.57	5.335	5.345	4.538	3.555	3.949	2.961
H3CS	1.87	2.617	2.617	2.043	1.477	1.849	0.734
H2CS	0.47	3.645	3.653	3.461	2.660	3.046	1.404
CH2CHO	1.82	4.955	4.924	4.347	3.651	4.029	2.563
CH3CO	0.42	2.906	2.903	2.336	1.734	2.123	0.951
H5C2O	1.71	5.224	5.217	4.511	3.495	3.882	2.879
HLi	0.34	1.619	1.022	0.464	1.130	1.428	-0.907
HNO	0.34	4.429	4.417	4.175	2.989	3.395	2.160
HO2	1.08	4.815	4.826	4.221	3.165	3.567	2.390
CS	0.21	3.415	3.429	3.232	2.392	2.782	0.735
ClO	2.28	6.015	6.035	5.461	4.575	4.968	3.588
Na2	0.43	1.775	1.837	1.625	1.321	1.625	0.266
P2	0.59	3.434	3.473	3.361	2.651	3.027	0.847
COS	0.46	1.915	1.920	1.651	0.958	1.342	-0.778
CS2	0.90	2.826	2.846	2.682	2.046	2.420	0.293
N2O	0.22	1.565	1.555	1.320	0.474	0.869	-1.334
NH2 rad	0.77	4.535	4.479	3.570	2.827	3.215	1.813
CH3NO2	0.48	3.132	3.121	3.038	2.049	2.445	0.541
MAD		2.858	2.833	2.525	1.795	2.163	0.640

[a] Same references as Table S17. [b] With the LUMO shifted according to Eq. (21) of the article.

Table S21: Ionization potentials in eV. Theoretical values determined through the negative of the HOMO.

System	Exp.[a]	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[b]
1,1-Dichloroethylene	10.00	6.529	6.552	6.767	7.697	7.299	10.545
1,3-Cyclohexadiene	8.32	5.180	5.197	5.296	6.150	5.757	8.856
Acetaldehyde	10.24	5.949	5.983	6.234	7.542	7.148	9.840
Adenine	8.44	5.519	5.524	5.670	6.489	6.100	9.267
Bromobenzene	9.00	6.115	6.133	6.310	7.135	6.742	10.027
Chlorobenzene	9.07	6.194	6.209	6.375	7.214	6.821	10.120
Chloroethylene	10.20	6.495	6.519	6.717	7.657	7.259	10.504
Chloromethane	11.29	7.099	7.143	7.400	8.512	8.114	11.271
cis-Dichloroethylene	9.80	6.350	6.376	6.598	7.515	7.120	10.327
Cytosine	8.80	5.714	5.721	5.928	6.828	6.433	9.514
Ethylene	10.68	6.776	6.793	6.937	7.899	7.492	10.841
Fluorobenzene	9.22	6.217	6.222	6.393	7.262	6.866	10.137
Naphthalene	8.14	5.499	5.504	5.603	6.342	5.956	9.242
Norbornadiene	8.38	5.438	5.447	5.573	6.492	6.092	9.171
Pyrazine	9.63	5.855	5.900	6.171	7.367	6.972	9.736
Pyridazine	9.31	5.349	5.397	5.682	6.955	6.556	9.107
Pyrimidine	9.73	5.951	5.990	6.256	7.488	7.089	9.849
Styrene	8.48	5.707	5.714	5.821	6.603	6.214	9.505
Thiophene	8.86	5.898	5.910	6.072	6.916	6.515	9.748
trans-Dichloroethylene	9.80	6.327	6.355	6.577	7.500	7.106	10.301
Trichloroethylene	9.60	6.330	6.355	6.584	7.499	7.106	10.301
Uracil	9.68	6.271	6.287	6.594	7.960	7.553	10.218
1,2,4-Trimethylbenzene	8.50	5.583	5.597	5.707	6.525	6.136	9.359
Acetone	9.80	5.672	5.698	5.948	7.264	6.866	9.484
Aniline	7.72	4.983	5.001	5.147	5.982	5.592	8.608
Anisole	8.20	5.398	5.409	5.564	6.431	6.038	9.123
cis-Butene	9.32	5.811	5.839	5.983	6.912	6.517	9.660
Cyclohexene	9.09	5.761	5.788	5.939	6.859	6.464	9.597
Furan	8.90	5.686	5.697	5.828	6.703	6.303	9.483
m-Xylene	8.55	5.815	5.827	5.948	6.770	6.377	9.646
o-Xylene	8.56	5.817	5.829	5.944	6.768	6.376	9.648
Phenol	8.75	5.552	5.564	5.722	6.584	6.190	9.316
Propene	9.91	6.261	6.285	6.433	7.375	6.975	10.214
Pyrrole	8.23	5.165	5.178	5.303	6.156	5.757	8.832
trans-Butene	9.37	5.814	5.841	5.987	6.915	6.520	9.663
Trimethylethylene	8.69	5.527	5.554	5.689	6.609	6.217	9.305
CO2	13.78	9.084	9.099	9.462	10.723	10.319	13.640
Guanine	8.24	5.294	5.296	5.438	6.245	5.858	8.981
HC	10.23	5.947	5.974	6.414	7.466	7.073	9.828
H3C	9.84	5.423	5.438	5.934	6.825	6.428	9.159
H2N	11.14	7.270	7.362	7.554	8.825	8.435	11.538
HO	13.01	7.368	7.447	7.802	9.223	8.830	11.642
HSi	7.89	4.536	4.574	4.860	5.554	5.169	8.067
H2Si	9.15	5.864	5.942	6.059	6.890	6.507	9.789
H3Si	8.14	5.366	5.406	5.681	6.444	6.060	9.119
H2P	9.82	6.055	6.078	6.493	7.262	6.870	9.958
HS	10.37	6.229	6.306	6.492	7.487	7.093	10.240
NO	9.26	4.596	4.623	5.088	6.513	6.117	8.128
CN	13.60	9.382	9.417	9.644	10.778	10.374	14.021
OP	8.39	4.670	4.702	5.068	5.985	5.597	8.230
Cl2	11.50	7.430	7.474	7.765	8.859	8.460	11.676
C2	11.40	8.050	8.090	8.206	9.276	8.873	12.424
CF2	11.42	7.367	7.400	7.795	9.005	8.608	11.584

Table S21 – continued

CNO	11.76	7.690	7.725	8.051	9.133	8.735	11.980
NO2	9.59	6.583	6.593	7.178	8.535	8.133	10.596
O3	12.73	7.919	7.943	8.319	9.847	9.441	12.245
OF	12.78	7.146	7.206	7.558	9.301	8.905	11.347
O2S	12.35	8.037	8.061	8.405	9.610	9.208	12.388
OS2	10.58	6.953	6.982	7.217	8.198	7.800	11.073
HC2	11.61	7.374	7.434	7.608	8.581	8.184	11.627
H3C2	8.25	5.530	5.567	6.033	7.011	6.624	9.320
H3C3	8.67	5.148	5.165	5.593	6.386	5.996	8.816
H5C3	8.18	4.744	4.761	5.260	5.926	5.537	8.304
HCO	8.14	5.001	5.039	5.460	6.559	6.173	8.657
HCF	10.06	5.859	5.926	6.167	7.380	6.991	9.769
CH3O	10.73	6.064	6.143	6.435	7.828	7.442	10.039
H3CS	9.26	4.197	4.230	4.581	5.487	5.097	7.625
H2CS	9.38	5.546	5.595	5.738	6.769	6.375	9.356
CH2CHO	10.85	6.007	6.048	6.425	7.654	7.258	9.921
CH3CO	7.00	4.463	4.473	4.874	5.967	5.577	7.937
H5C2O	9.11	5.885	5.954	6.273	7.646	7.257	9.804
HLi	7.90	4.349	4.391	4.490	5.421	5.028	7.832
HNO	10.10	5.565	5.626	5.890	7.247	6.856	9.394
HO2	11.35	6.296	6.361	6.784	8.248	7.854	10.308
CS	11.33	7.424	7.494	7.817	8.945	8.548	11.700
ClO	10.95	6.351	6.411	6.679	8.061	7.666	10.371
Na2	4.98	3.146	3.205	3.160	3.628	3.279	6.288
P2	10.53	7.150	7.186	7.410	8.129	7.730	11.324
COS	11.18	7.485	7.513	7.778	8.702	8.304	11.723
CS2	10.07	6.827	6.864	7.076	7.873	7.489	10.928
N2O	12.89	8.394	8.411	8.693	9.847	9.447	12.811
NH2 rad	11.14	7.279	7.370	7.563	8.835	8.445	11.548
CH3NO2	11.08	6.958	6.982	7.323	8.800	8.396	11.073
MAD		3.651	3.619	3.370	2.340	2.734	0.583

[a] Same references as Table S18. [b] With the HOMO shifted according to Eq. (20) of the article.

Table S22: Band gaps in eV. Theoretical values determined through the LUMO minus the HOMO.

System	Exp.[a]	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[b]
1,1-Dichloroethylene	10.75	4.808	4.860	5.266	6.908	6.137	11.333
1,3-Cyclohexadiene	9.12	3.458	3.486	3.791	5.367	4.600	9.292
Acetaldehyde	11.43	3.930	3.986	4.543	6.735	5.949	10.188
Adenine	9.08	3.865	3.889	4.227	5.726	4.973	9.863
Bromobenzene	9.70	4.508	4.538	4.891	6.424	5.663	10.813
Chlorobenzene	9.82	4.607	4.635	4.975	6.524	5.762	10.946
Chloroethylene	11.49	5.072	5.125	5.556	7.214	6.439	11.583
Chloromethane	14.74	6.194	6.469	7.022	8.291	7.597	13.213
cis-Dichloroethylene	10.92	4.762	4.794	5.198	6.882	6.111	11.185
Cytosine	9.16	3.726	3.745	4.102	5.717	4.949	9.818
Ethylene	12.46	5.707	5.760	6.220	7.841	7.058	12.345
Fluorobenzene	10.09	4.699	4.721	5.064	6.630	5.863	11.039
Naphthalene	8.34	3.426	3.436	3.682	5.090	4.345	9.400
Norbornadiene	9.42	4.058	4.109	4.417	6.068	5.299	10.044
Pyrazine	9.70	3.232	3.286	3.684	5.704	4.932	9.447
Pyridazine	9.63	2.774	2.830	3.270	5.338	4.562	8.739
Pyrimidine	9.98	3.578	3.630	4.083	6.090	5.314	9.835
Styrene	8.73	3.661	3.683	3.958	5.408	4.658	9.752
Thiophene	10.03	4.513	4.522	4.838	6.396	5.621	10.688
trans-Dichloroethylene	10.62	4.587	4.637	5.021	6.706	5.937	11.018
Trichloroethylene	10.18	4.447	4.481	4.854	6.523	5.757	10.862
Uracil	9.89	3.891	3.921	4.373	6.480	5.699	10.270
1,2,4-Trimethylbenzene	9.57	4.590	4.642	4.926	6.390	5.643	10.653
Acetone	11.31	4.024	4.071	4.631	6.777	5.995	10.133
Aniline	8.85	3.922	3.959	4.282	5.795	5.038	9.662
Anisole	9.29	4.232	4.259	4.589	6.147	5.387	10.175
cis-Butene	11.54	5.448	5.490	5.941	7.564	6.796	11.621
Cyclohexene	11.16	5.128	5.357	5.755	7.460	6.574	11.463
Furan	10.66	4.829	4.866	5.159	6.769	5.995	10.927
m-Xylene	9.61	4.716	4.757	5.067	6.546	5.790	10.883
o-Xylene	9.68	4.811	4.850	5.155	6.644	5.889	10.977
Phenol	9.76	4.288	4.316	4.648	6.199	5.436	10.310
Propene	11.90	5.517	5.581	6.029	7.606	6.840	11.928
Pyrrole	10.61	5.043	5.086	5.399	6.907	6.151	10.882
trans-Butene	11.47	5.372	5.439	5.872	7.451	6.690	11.571
Trimethylethylene	10.93	5.040	5.127	5.532	6.976	6.259	11.116
CO2	17.58	8.783	8.828	9.594	11.620	10.834	16.398
Guanine	8.70	3.928	3.971	4.310	5.843	5.103	9.828
HC	8.99	0.577	0.685	1.570	3.591	2.814	6.883
H3C	9.76	2.479	2.578	3.792	5.198	4.428	8.508
H2N	10.37	2.739	2.886	3.988	6.001	5.223	9.727
HO	11.18	0.924	1.058	2.398	4.926	4.136	7.937
HSi	6.61	0.296	0.344	0.832	2.250	1.497	5.816
H2Si	8.03	1.802	1.891	2.181	3.748	2.994	8.073
H3Si	6.73	1.818	1.896	2.623	3.850	3.097	7.810
H2P	8.55	1.845	1.857	2.778	4.140	3.374	8.106
HS	8.01	0.435	0.489	1.211	2.974	2.198	6.846
NO	9.24	0.280	0.331	1.085	3.628	2.828	5.830
CN	9.74	1.710	1.687	2.496	4.357	3.558	9.383
OP	7.30	0.181	0.210	0.701	2.454	1.679	5.752
Cl2	9.11	2.762	2.797	3.175	5.260	4.474	9.688
C2	8.13	0.907	0.934	0.162	2.242	1.446	8.090
CF2	11.24	3.627	3.702	4.242	6.506	5.714	10.560

Table S22 – continued

CNO	8.15	0.420	0.470	1.234	3.230	2.449	7.470
NO2	7.32	1.421	1.434	2.345	4.519	3.720	7.926
O3	10.63	1.825	1.851	2.155	4.688	3.882	8.944
OF	10.51	0.582	0.649	1.723	4.534	3.738	7.421
O2S	11.24	3.361	3.377	3.725	5.827	5.031	10.521
OS2	8.70	1.976	1.980	2.177	3.939	3.159	8.651
HC2	8.64	1.005	1.097	1.907	3.631	2.832	7.971
H3C2	7.58	2.372	2.415	3.645	5.134	4.368	8.410
H3C3	7.78	1.528	1.559	2.571	3.909	3.151	7.348
H5C3	7.71	1.497	1.533	2.730	3.866	3.110	7.107
HCO	7.83	1.696	1.679	2.633	4.468	3.679	7.402
HCF	9.52	1.618	1.734	2.191	4.464	3.683	7.909
CH3O	9.16	0.729	0.798	1.897	4.274	3.493	7.078
H3CS	7.39	1.580	1.613	2.538	4.010	3.248	6.891
H2CS	8.91	1.901	1.943	2.278	4.109	3.329	7.953
CH2CHO	9.03	1.052	1.124	2.078	4.003	3.229	7.357
CH3CO	6.58	1.557	1.570	2.538	4.233	3.454	6.986
H5C2O	7.40	0.660	0.737	1.763	4.150	3.375	6.925
HLi	7.56	2.730	3.369	4.026	4.291	3.599	8.739
HNO	9.76	1.137	1.209	1.715	4.258	3.461	7.234
HO2	10.27	1.481	1.535	2.563	5.082	4.287	7.918
CS	11.12	4.009	4.065	4.585	6.553	5.766	10.965
ClO	8.67	0.336	0.376	1.217	3.486	2.698	6.783
Na2	4.55	1.371	1.368	1.534	2.307	1.654	6.022
P2	9.94	3.716	3.714	4.049	5.478	4.703	10.477
COS	10.72	5.569	5.593	6.127	7.744	6.963	12.501
CS2	9.17	4.001	4.018	4.393	5.827	5.069	10.636
N2O	12.67	6.828	6.855	7.373	9.373	8.578	14.145
NH2 rad	10.37	2.744	2.891	3.993	6.008	5.230	9.735
CH3NO2	10.60	3.826	3.861	4.285	6.750	5.951	10.532
MAD		6.509	6.451	5.894	4.125	4.896	0.913

[a] Values from Table S17 and Table S18. [b] With the LUMO and HOMO shifted according to Eqs. (20) and (21) of the article.

Table S23: Semiconductors with small values of the band gap (in eV).

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[a]
AlSb	1.69	1.21	1.28	1.37	2.33	1.70	2.90
B	2.00	1.01	1.47	1.09	2.18	1.50	3.01
CdSe	1.74	0.75	0.52	1.07	2.32	1.72	2.19
CdSe	1.73	0.77	0.65	1.10	2.32	1.74	2.25
GaAs	1.52	0.57	0.53	0.80	2.07	1.46	2.14
GaSb	0.82	0.16	0.27	0.16	1.55	0.96	1.87
Ge	0.74	0.11	0.07	0.14	1.48	0.86	1.61
InAs	0.42	0.00	0.17	0.01	1.12	0.55	1.74
InN	0.70	0.00	0.49	0.02	1.35	0.74	2.00
InP	1.42	0.71	0.66	1.05	2.14	1.52	2.18
InSb	0.24	0.00	0.24	0.00	0.97	0.54	1.75
ScN	0.90	0.00	0.01	0.30	1.59	0.91	1.53
Si	1.17	0.62	0.77	0.87	1.83	1.20	2.32
SnSe	0.90	0.60	0.68	0.82	1.55	1.03	2.33
SnTe	0.36	0.09	0.33	0.08	0.64	0.10	1.84
MAD		0.65	0.55	0.50	0.61	0.12	1.02

[a] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S24: Layered solids band gap (in eV).

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[a]
HfS2	1.96	1.00	1.24	1.27	2.37	1.81	2.84
HfSe2	1.13	0.47	0.59	0.75	1.76	1.16	2.19
MoS2	1.23	0.90	1.27	0.99	2.09	1.47	2.79
MoSe2	1.09	0.81	1.46	0.94	1.92	1.31	3.16
TiO2	3.03	2.16	1.77	2.50	4.27	3.66	3.35
TiO2-390	3.30	2.06	2.09	2.43	4.20	3.55	3.67
WS2	1.35	1.00	1.61	1.11	2.16	1.53	3.40
WSe2	1.20	0.95	1.49	1.10	2.00	1.43	3.21
ZrS2	1.68	0.80	1.13	1.16	2.15	1.58	2.91
ZrSe2	1.18	0.36	0.41	0.72	1.59	1.02	2.10
ZnS	3.72	2.15	2.06	2.63	4.04	3.38	3.62
MAD		0.75	0.70	0.48	0.70	0.23	1.14

[a] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S25: Semiconductors with intermediate values of the band gap (in eV).

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[a]
AgBr	2.71	0.72	0.79	1.16	2.66	2.05	2.42
AgCl	3.25	0.93	1.03	1.39	3.06	2.43	2.56
AgF	2.80	0.00	0.00	0.00	2.05	1.34	1.51
AgI	3.02	1.49	1.38	1.76	3.14	2.60	2.98
AgI	2.91	1.36	1.35	1.66	3.13	2.50	2.86
AlAs	2.23	1.43	1.66	1.73	2.71	2.07	3.20
AlN	6.11	4.14	4.15	4.79	6.17	5.50	5.67
AlP	2.45	1.58	1.80	1.90	2.95	2.28	3.32
BaS	3.81	2.10	2.22	2.45	3.56	3.03	3.74
BaSe	3.42	1.88	2.02	2.24	3.35	2.71	3.69
BaTe	3.40	1.52	1.67	1.85	2.81	2.19	3.22
BP	2.10	1.27	1.33	1.58	2.69	2.02	2.97
C	5.50	4.15	4.18	4.57	6.10	5.34	5.85
CdS	2.48	1.24	1.10	1.59	2.91	2.29	2.75
Cu2O	2.17	0.53	0.50	0.77	2.66	2.02	2.25
CuBr	3.07	0.48	0.58	0.74	2.79	2.18	2.20
CuCl	3.40	0.54	0.65	0.81	2.94	2.35	2.25
CuI	3.12	1.18	1.27	1.49	3.28	2.64	3.13
GaN	3.50	1.87	1.74	2.23	3.83	3.15	3.35
GaP	2.35	1.64	1.62	1.88	2.93	2.30	3.14
LiH	4.94	3.00	3.21	3.64	4.66	3.99	5.01
MgTe	3.49	2.57	2.45	3.18	3.90	3.39	4.14
SiC	3.23	2.23	2.32	2.60	3.88	3.17	3.88
SiC-7140	3.33	2.35	2.48	2.72	3.83	3.26	4.04
SiC-7631	3.20	2.01	2.13	2.37	3.64	2.92	3.74
SiC-8062	2.42	1.35	1.48	1.71	2.98	2.25	3.20
ZnO	3.44	0.80	0.76	1.14	3.14	2.51	2.36
ZnSe	2.82	1.31	1.29	1.71	3.04	2.42	2.86
BN	6.36	4.45	4.52	4.93	6.56	5.79	6.16
MAD		1.62	1.56	1.26	0.37	0.49	0.50

[a] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S26: Ionic solids band gap (in eV).

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[a]
BeO	10.59	7.35	7.56	8.16	9.96	9.23	9.48
CaO	6.88	3.63	3.70	4.16	6.01	5.31	5.24
Kbr	7.80	4.36	4.38	4.91	6.23	5.51	5.95
Kcl	8.69	5.21	5.11	5.78	6.82	6.52	6.75
LiCl	9.40	6.33	6.42	7.18	8.28	7.74	8.24
LiF	13.60	9.08	8.80	9.98	11.94	11.39	10.49
MgO	7.67	4.71	4.54	5.53	7.14	6.44	6.24
NaBr	7.10	4.13	4.24	4.83	5.80	5.32	5.88
NaI	5.80	3.63	3.71	4.35	5.09	4.62	5.31
NaCl	8.75	5.10	5.16	5.85	7.01	6.46	6.72
NaF	11.70	6.31	6.21	7.02	8.99	8.41	7.81
MAD		3.47	3.47	2.75	1.34	1.91	1.81

[a] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S27: Insulator solids band gap (in eV).

System	Exp.	PBE	NCAPR	SCAN	PBE0	HSE06	NCAPR[a]
Ar	14.15	8.71	8.94	9.50	10.69	10.34	10.54
Kr	11.59	7.27	7.69	8.04	9.42	8.67	9.30
Ne	21.48	11.58	12.43	12.77	15.12	14.30	14.08
Xe	9.29	6.26	6.38	6.93	7.92	7.38	7.90
MAD		5.67	5.27	4.82	3.34	3.95	3.67

[a] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S28: Comparison of the results for solids in eV with the test set reported in Ref. [62].

System	Exp.	LDA	PBE	NCAPR	HSE06	SCAN	SCAN gKS[a]	MS2 gKS[b]	MVS gKS[c]	NCAPR[d]
Si	1.17	0.60	0.71	0.77	1.11	0.78	0.97	1.20	1.04	2.32
InP	1.42	0.50	0.72	0.66	1.52	0.77	1.06	1.14	1.99	2.18
GaAs	1.52	0.30	0.53	0.53	1.41	0.45	0.80	0.94	2.15	2.14
BaS	1.6	1.21	1.26	0.00	1.71	1.32	1.51	1.63	1.56	0.00
CdSe	1.73	0.44	0.71	0.52	1.66	0.76	1.10	1.06	2.14	2.19
BP	2.1	1.36	1.43	1.33	1.79	1.52	1.74	1.94	1.64	2.97
GaP	2.35	1.53	1.69	1.62	2.09	1.72	1.94	1.97	2.23	3.14
CdS	2.48	0.96	1.23	1.10	2.27	1.20	1.62	1.60	2.39	2.75
B-GaN	3.17	1.70	1.69	0.00	2.97	1.84	2.03	1.69	2.50	0.00
ZnS	3.72	1.87	2.12	2.06	3.32	2.16	2.63	2.52	3.35	3.62
C	5.5	4.14	4.17	4.18	4.94	4.26	4.58	4.79	4.15	5.85
BN	6.2	4.42	4.53	4.52	5.39	4.73	5.04	5.01	5.14	6.16
CaO	6.93	3.62	3.75	3.70	5.30	3.78	4.29	4.13	4.56	5.24
MgO	7.9	4.70	4.74	4.54	6.46	4.80	5.62	5.20	6.05	6.24
NaCl	8.97	4.70	5.08	5.16	6.42	5.25	5.86	5.85	6.61	6.72
LiF	13.6	8.84	9.04	8.80	11.40	9.11	9.97	9.50	10.64	10.49
Ar	14.3	8.44	8.92	8.94	10.33	8.89	9.91	9.95	10.98	10.54
MAD		2.08	1.90	2.10	0.88	1.84	1.41	1.29	1.13	1.19

[a] SCAN in a generalized Kohn-Sham scheme, see Ref. 62.
[b] meta-GGA Made Simple 2 [J. Sun, B. Xiao, and A. Ruzsinszky, J. Chem. Phys. 137, 051101 (2012); J. Sun, R. Haunschild, B. Xiao, I. W. Bulik, G. E. Scuseria, and J. P. Perdew, J. Chem. Phys. 138, 044113 (2013)].
[c] meta-GGA made very simple [J. Sun, J. P. Perdew, and A. Ruzsinszky, Proc. Natl. Acad. Sci. USA 112, 685 (2014)].
[d] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S29: Comparison of the results for solids in eV with the test set reported in Ref. [13].

System	Exp.	HF	LDA	NCAPR	B3LYP	MLDA[a]	NCAPR[b]
AlAs	2.23	2.71	1.75	1.66	12.70	2.17	3.20
AlP	2.51	8.00	1.91	1.80	7.22	2.40	3.32
BAs	1.46	5.83	1.15	0.00	3.52	1.46	0.00
BP	2.00	7.15	1.30	1.33	3.75	1.75	2.97
C	5.48	8.07	4.06	4.18	8.27	5.05	5.85
GaAs	1.52	1.75	1.59	0.53	10.38	1.98	2.14
GaN	3.50	7.61	2.70	1.74	7.24	3.43	3.35
GaP	2.35	7.29	1.93	1.62	5.80	2.39	3.14
Ge	0.74	5.56	0.49	0.07	3.09	0.76	1.61
LiCl	9.40	3.05	6.35	6.42	25.55	7.61	8.24
MgO	7.90	2.85	6.09	4.54	19.43	8.26	6.24
NaCl	8.50	8.70	5.10	5.16	9.15	6.40	6.72
NaF	11.60	8.21	6.68	6.21	14.77	9.79	7.81
Ne	21.50	3.02	11.51	12.43	6.30	16.39	14.08
Si	1.17	0.79	0.63	0.77	11.10	1.00	2.32
SiC	2.42	1.51	1.59	1.48	17.72	2.13	3.20
ZnO	3.44	2.96	1.71	0.76	14.42	3.00	2.36
ZnS	3.78	2.71	2.50	2.06	15.83	3.25	3.62
MAD		11.22	1.81	2.19	0.99	0.77	1.44

[a] Modified Local Density Approximation see Ref. 13.
[b] With the frontier eigenvalues shifted according to Eqs. (20) and (21)

Table S30: Comparison of the results for solids in eV with the test set reported in Ref. [61].

System	Exp.	NCAPR	SCAN	SCAN-L[a]	NCAPR[b]
AlAs	2.23	1.66	1.74	1.59	3.20
AlN	4.90	4.15	3.97	3.50	5.67
AlP	2.50	1.80	1.92	1.81	3.32
BN	6.36	4.52	4.98	4.66	6.16
BP	2.10	1.33	1.54	1.41	2.97
C	5.50	4.18	4.54	4.22	5.85
GaAs	1.52	0.53	0.77	0.33	2.14
GaN	3.28	1.74	1.96	1.49	3.35
GaP	2.35	1.62	1.83	1.72	3.14
Ge	0.74	0.07	0.14	0.00	1.61
InAs	0.42	0.17	0.00	0.00	1.74
InP	1.42	0.66	1.02	0.59	2.18
InSb	0.24	0.24	0.00	0.00	1.75
LiCl	9.40	6.42	7.33	6.80	8.24
LiF	14.20	8.80	10.10	9.16	10.49
LiH	4.94	3.21	3.66	3.69	5.01
MgO	7.83	4.54	5.79	4.92	6.24
NaCl	8.50	5.16	5.99	5.59	6.72
NaF	11.50	6.21	7.14	6.45	7.81
Si	1.17	0.77	0.82	0.80	2.32
SiC	2.42	1.48	1.72	1.55	3.20
MAD		1.63	1.26	1.58	1.14

[a] SCAN with the kinetic energy density described in terms of the Laplacian of the density, see Ref. 61.
[b] With the frontier eigenvalues shifted according to Eqs. (20) and (21)