Suplementary information for: Generalized Gradient Approximation Exchange Energy Functional with Correct Asymptotic Behavior of the Corresponding Potential.

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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: 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	$\Delta_f H^o_{298}$	LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	LiH	33.3	-2.3	5.0	0.4	1.7	5.7	2.3	7.8
2	BeH	81.7	-9.3	-4.7	-5.9	-4.4	-3.9	-5.3	-4.3
3	CH	142.5	-8.3	-0.6	-1.5	-0.6	0.7	-0.3	1.8
4	$CH_2(^3B_1)$	93.7	-22.3	-4.1	0.3	-3.1	-0.2	0.8	-1.8
5	$CH_2(^1A_1)$	102.8	-17.5	2.2	1.2	1.1	5.9	2.8	6.3
6	CH_3	35.0	-31.6	-2.5	0.5	-2.4	3.4	2.0	2.5
7	CH_4	-17.9	-42.1	0.0	3.1	-1.5	8.5	4.8	6.4
8	NH	85.2	-11.3	-4.5	-5.5	-2.4	-3.2	-3.7	-1.2
9	NH_2	45.1	-25.2	-6.1	-6.9	-3.3	-2.3	-4.4	-0.4
10	NH_3	-11.0	-38.0	-2.9	-2.6	-1.1	4.2	-0.3	4.1
11	OH	9.4	-16.9	-2.7	-2.5	-1.3	0.1	-1.8	-0.4
12	H_2O	-57.8	-32.4	-0.4	1.3	0.1	6.3	1.6	3.1
13	FH	-65.1	-20.0	0.1	1.1	-0.8	4.2	0.7	1.2
14	$SiH_2(^1A_1)$	65.2	-14.6	3.5	-0.5	-0.1	6.6	0.7	5.9
15	$SiH_2(^3B_1)$	86.2	-16.4	-1.1	0.1	-4.4	2.0	0.0	-0.6
16	SiH_3	47.9	-21.4	2.9	0.9	-1.8	7.3	2.0	5.4
17	SiH_4	8.2	-25.3	8.3	4.0	2.4	14.3	6.0	12.5
18	PH_2	33.1	-20.7	-1.6	-4.6	-3.8	1.9	-3.5	0.9
19	PH_3	1.3	-27.8	2.7	-0.6	-0.8	8.3	0.6	6.1
20	H_2S	-4.9	-23.7	0.5	1.8	-1.2	5.4	1.5	2.2
21	HCl	-22.1	-13.8	0.1	2.1	-1.0	3.1	1.4	0.6
22	Li_2	51.6	1.0	4.6	4.2	3.1	5.0	7.1	9.9
23	LiF	-80.1	-16.3	0.9	-0.6	4.1	4.0	3.1	7.7
24	HCCH	54.2	-53.7	-8.9	0.9	1.2	1.1	3.3	1.2
25	CH_2CH_2	12.5	-68.7	-8.1	2.7	-0.8	5.1	5.6	3.9
26	CH_3CH_3	-20.1	-81.7	-4.9	7.4	-0.1	11.6	10.6	8.8
27	CN	104.9	-37.5	-15.8	-9.6	-3.1	-10.6	-6.8	-7.1
28	HCN	31.5	-47.4	-13.2	-7.2	-1.0	-5.5	-3.8	-2.7
29	CO	-26.4	-39.4	-9.6	-2.6	-0.1	-2.7	-1.4	-3.1
30	CHO	10.0	-53.9	-16.4	-8.3	-7.1	-7.8	-6.9	-8.8
31	CH_2O	-26.0	-59.7	-12.0	-3.9	-4.3	-1.6	-2.1	-3.3
32	CH_3OH	-48.0	-72.9	-6.9	2.4	-0.5	7.5	4.6	4.0
33	N_2	0.0	-38.2	-14.7	-11.4	-0.4	-9.4	-7.4	-4.2

Table S1 – continued

34	N_2H_4	22.8	-75.6	-13.4	-7.7	-2.1	0.1	-3.0	1.4
35	NO	21.6	-45.7	-19.3	-13.6	-7.6	-13.0	-11.7	-11.6
36	O_2	0.0	-54.6	-23.6	-15.4	-16.2	-16.2	-15.9	-19.1
37	H_2O_2	-32.5	-65.3	-12.7	-6.1	-4.0	-1.0	-4.9	-4.6
38	F_2	0.0	-39.7	-14.5	-10.2	-8.4	-8.6	-10.1	-10.8
39	CO_2	-94.1	-83.6	-27.1	-10.6	-9.5	-13.6	-9.6	-16.6
40	Na_2	34.0	-3.3	-0.7	-0.7	-3.1	-0.5	3.5	7.6
41	Si_2	139.9	-16.2	-6.7	1.4	-2.0	-3.6	1.7	-4.3
42	P_2	34.3	-25.8	-4.2	-4.2	1.7	0.6	-3.1	-0.0
43	S_2	30.7	-33.5	-13.7	-6.1	-7.5	-8.7	-6.6	-11.1
44	Cl_2	0.0	-25.0	-7.9	-0.5	-2.2	-3.3	-1.0	-5.7
45	NaCl	-43.6	-5.4	4.1	6.7	6.2	6.4	8.4	7.3
46	SiO	-24.6	-30.7	-3.2	-2.2	4.8	2.9	-0.0	2.8
47	CS	66.9	-30.4	-8.3	-1.0	-0.7	-2.9	-0.5	-3.5
48	SO	1.2	-41.6	-15.5	-9.3	-8.0	-9.2	-9.0	-11.3
49	ClO	24.2	-38.8	-16.3	-9.8	-8.4	-10.8	-9.6	-12.3
50	ClF	-13.2	-33.2	-10.7	-5.5	-4.8	-5.2	-5.4	-7.4
51	Si_2H_6	19.1	-49.0	10.1	9.8	6.3	21.6	13.2	18.7
52	CH_3Cl	-19.6	-52.2	-5.5	4.6	-0.6	4.9	5.7	2.2
53	CH_3SH	-5.5	-62.4	-4.7	5.6	-0.1	7.9	6.9	4.2
54	HOCl	-17.8	-45.8	-10.6	-3.8	-3.4	-2.4	-3.4	-5.3
55	SO_2	-71.0	-75.5	-20.6	-6.5	-4.6	-7.3	-6.0	-11.8
56	BF_3	-271.4	-77.7	-11.0	2.1	6.6	4.7	5.9	3.2
57	BCl_3	-96.3	-59.3	-13.6	9.9	4.6	-1.3	10.4	-3.8
58	AlF_3	-289.0	-54.7	0.6	6.3	12.9	12.9	11.7	14.1
59	$AlCl_3$	-139.7	-37.5	-0.9	15.8	12.5	8.9	17.4	7.4
60	CF_4	-223.0	-122.9	-27.9	-1.0	-3.8	-4.4	0.2	-11.3
61	CCl4	-22.9	-87.8	-21.5	12.7	6.3	-3.3	12.8	-7.7
62	COS	-33.1	-75.3	-26.2	-9.9	-10.1	-14.2	-9.4	-17.3
63	CS_2	28.0	-65.8	-23.8	-7.3	-9.3	-13.2	-7.3	-16.5
64	COF_2	-149.1	-100.8	-25.3	-3.7	-4.5	-6.9	-2.7	-11.9
65	SiF_4	-386.0	-80.9	2.3	13.9	22.1	21.7	19.6	19.9
66	SiCl4	-158.4	-59.7	-3.6	24.1	17.8	11.7	24.9	7.7
67	N_2O	19.6	-90.7	-40.2	-26.1	-18.1	-28.0	-23.2	-26.3
68	NOCl	12.4	-74.7	-33.3	-21.8	-15.8	-23.2	-19.7	-22.6
69	NF_3	-31.6	-107.0	-40.3	-23.5	-19.0	-23.9	-21.5	-26.0
70	PF_3	-229.1	-77.5	-10.3	-1.2	6.4	5.5	2.3	2.9

Table S1 – continued

71	O_3	34.1	-95.0	-37.8	-22.4	-19.7	-24.0	-22.5	-28.2
72	F_2O	5.9	-78.0	-30.6	-20.7	-16.5	-19.2	-19.9	-22.1
73	ClF_3	-38.0	-102.2	-39.5	-23.8	-20.3	-24.0	-22.4	-27.9
74	CF_2CF_2	-157.4	-160.9	-47.3	-12.8	-13.7	-19.2	-10.4	-25.6
75	CCl_2CCl_2	-3.0	-122.3	-35.0	9.4	1.9	-11.4	10.0	-16.2
76	CF_3CN	-118.4	-150.1	-41.9	-9.5	-4.1	-15.2	-4.5	-16.2
77	CH_3CCH(propyne)	44.2	-96.3	-15.8	3.6	0.6	2.4	7.4	1.2
78	CH_2CCH_2(allene)	45.5	-101.4	-20.6	-1.0	-4.1	-2.3	2.8	-3.4
79	$C3H_4$(cyclopropene)	66.2	-101.4	-18.7	6.1	-2.5	0.4	8.2	-2.7
80	CH_3CHCH_2(propylene)	4.8	-109.8	-13.3	7.2	0.8	8.1	11.6	6.2
81	$C3H_6$(cyclopropane)	12.7	-115.0	-15.4	10.6	-1.0	7.2	13.4	2.9
82	$C3H_8$(propane)	-25.0	-121.4	-9.0	12.9	2.8	15.7	17.8	12.6
83	C_4H_6(1,3-butadien)	26.3	-137.8	-22.2	6.4	1.1	4.2	12.2	3.2
84	C_4H_6(2-butyne)	34.8	-137.7	-21.7	7.5	1.1	4.7	12.5	2.3
85	C_4H_6(methylene cyclopropane)	47.9	-147.1	-28.0	6.3	-4.8	-0.5	10.1	-4.4
86	C_4H_6(bicyclobutane)	51.9	-147.2	-25.0	15.3	-1.3	3.8	17.5	-2.1
87	C_4H_6(cyclobutene)	37.4	-142.7	-22.7	12.9	1.3	5.4	16.5	0.8
88	C_4H_8(cyclobutane)	6.8	-154.9	-19.1	17.1	2.9	12.1	21.5	6.7
89	C_4H_8(isobutene)	-4.0	-150.2	-17.4	13.2	4.2	12.5	19.3	10.2
90	C_4H_{10}(butane)	-30.0	-160.9	-12.9	18.6	5.9	20.0	25.2	16.6
91	C_4H_{10}(isobutane)	-32.1	-160.8	-11.9	19.9	7.6	21.2	26.8	18.2
92	C_5H_8(spiropentane)	44.3	-189.8	-32.0	17.3	-1.6	4.9	21.2	-1.7
93	C_6H_6(benzene)	19.7	-205.4	-42.2	10.9	2.9	-2.9	17.4	-6.3
94	CH_2F_2	-107.7	-80.5	-14.4	-1.2	-3.4	0.8	0.7	-2.9
95	CHF_3	-166.6	-101.6	-21.3	-1.5	-3.7	-2.0	0.2	-7.0
96	CH_2Cl_2	-22.8	-63.4	-11.0	6.7	0.8	1.8	7.4	-1.5
97	$CHCl_3$	-24.7	-75.3	-16.4	9.4	3.1	-0.9	9.8	-4.8
98	CH_3NH_2(methylamine)	-5.5	-77.8	-8.1	0.7	-0.2	6.9	4.7	6.1
99	CH_3CN(acetronitrile)	18.0	-89.6	-19.8	-4.2	-1.3	-3.9	0.5	-2.3
100	CH_3NO_2(nitromethane)	-17.8	-142.1	-41.0	-16.7	-14.8	-17.3	-13.0	-19.9
101	CH_3ONO(methyl nitrite)	-15.9	-137.5	-38.7	-16.7	-12.0	-15.6	-12.2	-16.9
102	CH_3SiH_3(methyl silane)	-7.0	-63.0	5.2	10.5	5.8	19.2	14.0	16.7
103	HCOOH(formic acid)	-90.5	-96.2	-21.3	-5.1	-5.0	-4.1	-3.0	-7.7
104	$HCOOCH_3$(methyl formate)	-85.0	-136.6	-26.7	-2.6	-3.2	-1.4	1.7	-5.0
105	CH_3CONH_2(acetamide)	-57.0	-142.0	-26.9	-2.0	-1.7	-0.6	3.8	-2.0
106	C_2H_4NH(aziridine)	30.2	-110.7	-19.9	2.3	-2.9	1.0	5.9	-1.2
107	C_2N_2(cyanogen)	73.3	-97.0	-35.8	-17.9	-4.0	-21.1	-11.2	-14.3

Table S1 – continued

108	$(CH_3)_2NH$(dimethylamine)	-4.4	-118.6	-13.0	4.9	1.9	10.2	10.8	9.3
109	$CH_3CH_2NH_2$(ethylamine)	-11.3	-118.9	-13.5	4.9	1.4	9.7	10.7	8.7
110	CH_2CO(ketene)	-11.4	-94.7	-25.7	-7.7	-8.4	-9.7	-5.3	-11.8
111	C_2H_4O(oxirane)	-12.6	-105.7	-19.3	2.7	-4.3	0.6	4.6	-4.1
112	CH_3CHO(acetaldehyde)	-39.7	-101.4	-17.6	0.2	-3.1	1.2	3.6	-1.2
113	HCOCHO(glyoxal)	-50.7	-118.7	-29.7	-7.1	-5.7	-8.9	-3.3	-10.6
114	CH_3CH_2OH(ethanol)	-56.2	-113.0	-11.1	7.6	2.1	11.5	11.6	7.7
115	CH_3OCH_3(dimethyl ether)	-44.0	-113.7	-12.2	5.3	0.9	10.2	9.7	7.0
116	C_2H_4S(thiirane)	19.6	-95.5	-16.4	7.2	-2.4	2.1	8.4	-2.9
117	$(CH_3)_2SO$(dimethyl sulfoxide)	-36.2	-135.9	-18.7	8.3	0.9	8.0	12.3	3.3
118	C_2H_5SH(ethanethiol)	-11.1	-101.8	-8.5	11.4	3.1	12.4	14.4	8.2
119	CH_3SCH_3(dimethyl sulfide)	-8.9	-101.9	-9.8	10.0	1.5	10.8	13.1	6.9
120	CH_2CHF(vinil fluoride)	-33.2	-91.6	-17.9	-1.4	-4.1	-1.1	1.4	-3.4
121	C_2H_5Cl(ethyl chloride)	-26.8	-92.0	-9.7	9.9	2.2	9.0	12.8	5.9
122	CH_2CHCl(vinyl chloride)	8.9	-85.2	-18.5	0.3	-4.4	-3.0	2.5	-5.1
123	CH_2CHCN(acrylonitrile)	43.2	-115.3	-26.9	-3.7	0.4	-6.4	2.4	-3.7
124	CH_3COCH_3(acetone)	-51.9	-141.9	-21.8	5.8	-0.1	5.4	10.8	2.5
125	CH_3COOH(acetic acid)	-103.4	-136.2	-25.2	0.6	-1.9	0.5	4.3	-3.9
126	CH_3COF(acetyl fluoride)	-105.7	-123.0	-25.3	-1.2	-4.0	-2.6	2.0	-6.4
127	CH_3COCl(acetyl chloride)	-58.0	-115.5	-25.4	0.3	-3.5	-4.0	3.1	-7.3
128	$CH_3CH_2CH_2Cl$(propyl chloride)	-31.5	-131.8	-13.9	15.3	5.0	13.0	19.9	9.5
129	$(CH_3)_2CHOH$(isopropanol)	-65.2	-153.2	-14.8	13.8	6.0	16.3	19.7	12.4
130	$C_2H_5OCH_3$(methyl ethyl ether)	-51.7	-154.1	-16.8	10.1	3.2	13.9	16.3	10.2
131	$(CH_3)_3N$(trimethylamine)	-5.7	-160.0	-17.5	10.0	5.4	14.3	18.0	13.6
132	C_4H_4O(furan)	-8.3	-171.0	-37.7	4.3	-1.4	-5.5	8.1	-11.0
133	C_4H_4S(thiophene)	27.5	-158.1	-34.1	10.0	0.6	-3.7	12.9	-9.4
134	C_4H_5N(pyrrole)	25.9	-177.6	-39.3	3.3	-0.8	-6.0	8.7	-9.2
135	C_5H_5N(pyridine)	33.6	-202.2	-47.6	1.5	-0.2	-10.2	9.0	-11.2
136	H_2	0.0	-3.5	4.9	0.1	-2.2	5.8	-0.0	4.2
137	SH	34.2	-12.6	-1.0	-0.8	-1.6	1.3	-0.7	-0.0
138	$CCH(^2A',C_s)$	135.1	-42.9	-11.2	-0.5	-0.6	-3.6	1.2	-3.4
139	$CHCH_2(^2A',C_s)$	71.6	-62.1	-13.1	-1.9	-4.3	-2.1	0.6	-2.6
140	$CH_3CO(^2A',C_s)$	-2.4	-95.2	-22.2	-4.7	-6.5	-5.5	-1.7	-7.1
141	$CH_2OH(^2A,C_1)$	-4.1	-67.2	-11.7	-2.1	-3.6	0.7	-0.2	-2.0
142	$CH_3O(^2A',C_s)$	4.1	-59.8	-12.4	-4.0	-5.0	-1.1	-1.7	-2.7
143	$CH_3CH_2O(^2A'',C_s)$	-3.7	-100.2	-18.4	-0.6	-4.3	1.1	3.4	-0.8
144	$CH_3S(^2A',C_s)$	29.8	-53.2	-8.4	1.1	-2.5	1.9	2.6	-0.3

Table S1 – continued

145	$CH_3CH_2(^2A'$,$C_s)$	28.9	-73.8	-8.8	3.5	-2.3	5.4	6.5	3.5
146	$(CH_3)_2CH(^2A'$,$C_s)$	21.5	-115.6	-14.5	7.4	-1.3	7.9	12.0	5.5
147	$(CH_3)_3C$(t-butyl radical C_{3v})	12.3	-156.1	-18.5	13.4	2.1	12.5	19.7	9.6
148	NO_2	7.9	-95.8	-42.5	-27.1	-22.9	-29.5	-25.7	-30.8
149	CH_2=C=$CHCH_3$ (1,2-butadiene)	38.8	-141.2	-25.1	4.0	-2.0	1.4	9.3	-0.5
150	CH_2=CH-$C(CH_3)$=CH_2 (isoprene)	18.0	-178.4	-25.8	13.1	5.7	9.2	20.7	7.9
151	C_5H_{10} (cyclopentane)	-18.3	-194.4	-20.9	25.7	9.8	19.3	32.0	13.4
152	C_5H_{12} (n-pentane)	-35.1	-200.3	-16.6	24.5	9.2	24.5	32.9	20.7
153	$C(CH_3)_4$ (neopentane)	-40.2	-199.8	-13.6	28.6	14.5	28.3	37.5	25.3
154	C_6H_8 (1,3-cyclohexadiene)	25.4	-213.3	-34.7	19.1	8.5	7.6	26.3	3.5
155	C_6H_8 (1,4-cyclohexadiene)	25.0	-212.9	-34.2	19.8	8.9	8.2	26.8	3.7
156	C_6H_{12} (cyclohexane)	-29.5	-234.8	-23.6	33.0	16.0	25.4	41.5	19.6
157	C_6H_{14} (n-hexane)	-39.9	-240.0	-20.7	30.0	12.2	28.7	40.1	24.5
158	C_6H_{14} (3-methyl pentane)	-41.1	-239.9	-18.8	32.6	16.0	31.1	43.2	27.6
159	$C_6H_5CH_3$ (toluene)	12.0	-245.6	-46.3	16.7	6.1	1.4	24.9	-2.6
160	C_7H_{16} (n-heptane)	-44.9	-279.4	-24.5	35.8	15.4	33.1	47.7	28.6
161	C_8H_8 (1,3,5,7-cyclooctatetraene)	70.7	-270.2	-51.8	18.5	11.2	0.7	28.7	-1.2
162	C_8H_{18} (n-octane)	-49.9	-318.9	-28.4	41.5	18.6	37.5	55.1	32.6
163	$C_{10}H_8$ (naphthalene)	35.9	-341.6	-75.4	20.0	8.4	-9.8	30.6	-14.8
164	$C_{10}H_8$ (azulene)	69.1	-343.1	-78.2	16.9	4.8	-13.1	27.4	-17.6
165	CH_3COOCH_3 (methyl acetate)	-98.4	-175.7	-29.5	4.2	1.1	4.2	10.1	-0.1
166	$(CH_3)_3COH$ (t-butanol)	-74.7	-192.7	-17.2	21.5	12.0	22.6	29.4	18.7
167	$C_6H_5NH_2$ (aniline)	20.8	-246.2	-52.6	7.5	3.2	-6.0	16.4	-8.3
168	C_6H_5OH (phenol)	-23.0	-239.9	-50.2	10.6	3.7	-4.3	17.6	-9.3
169	CH_2=CH-O-CH=CH_2 (divinyl ether)	-3.3	-173.7	-31.6	3.2	0.2	1.3	9.7	-1.3
170	C_4H_8O (tetrahydrofuran)	-44.0	-186.8	-24.4	17.7	7.3	13.5	23.3	7.2
171	C_5H_8O (cyclopentanone)	-45.9	-216.5	-35.4	16.9	4.9	7.3	23.2	1.3
172	$C_6H_4O_2$ (1,4-benzoquinone)	-29.4	25.3	-60.9	2.9	1.5	-14.1	10.9	-17.1
173	$C_4H_4N_2$ (pyrimidine)	46.8	-200.0	-54.1	-8.8	-4.4	-18.5	-0.5	-17.4
174	$(CH_3)_2SO_2$ (dimethyl sulfone)	-89.2	-168.3	-23.7	12.8	3.8	10.1	16.8	2.7
175	C_6H_5Cl (chlorobenzene)	12.4	-217.8	-48.2	13.0	4.1	-6.4	19.0	-10.6
176	NC-CH_2CH_2-CN (succinonitrile)	50.1	-174.6	-42.1	-4.7	3.2	-10.8	4.9	-5.6
177	$C_4H_4N_2$ (pyrazine)	46.9	-196.4	-50.5	-5.4	-0.8	-15.0	2.9	-13.7
178	CH_3COCCH (acetyl acetylene)	15.6	-153.3	-31.0	3.1	1.8	-2.4	8.9	-3.5
179	CH_3-CH=CH-CHO (crotonaledehyde)	-24.0	-171.6	-32.8	2.7	-2.2	-0.8	9.0	-3.0
180	$(CH_3CO)_2O$ (acetic anhydride)	-136.8	-237.9	-48.5	1.0	-1.5	-4.0	8.4	-9.0
181	C_4H_6S (25-dihydrothiophene)	20.8	-165.1	-27.5	15.7	5.1	5.4	19.6	-0.5

Table S1 – continued

182	$CH_3CH(CH_3)CN$ (2-methyl propanenitrile)	5.6	-165.9	-25.3	9.3	7.1	6.9	17.6	8.0
183	CH_3-CO-CH_2CH_3 (methyl ethyl ketone)	-57.1	-181.8	-25.7	11.6	3.4	9.9	18.4	6.5
184	$(CH_3)_2$CH-CHO (isobutyraldehyde)	-51.6	-178.9	-23.7	13.4	5.2	11.7	20.4	8.8
185	$C_4H_8O_2$ (1,4-dioxane)	-75.5	-220.9	-31.8	15.7	10.0	12.6	23.0	6.2
186	C_4H_8S (tetrahydrothiophene)	-8.2	-174.9	-21.0	23.5	9.7	15.2	28.1	8.5
187	$(CH_3)_3$C-Cl (t-butyl chloride)	-43.5	-171.6	-15.7	23.9	12.5	20.2	30.8	17.0
188	$CH_3CH_2CH_2CH_2Cl$ (n-butyl chloride)	-37.0	-170.6	-17.2	21.6	8.7	18.0	27.9	14.1
189	C_4H_8NH (pyrrolidine)	-0.8	-192.4	-25.8	16.7	7.9	13.0	24.0	9.2
190	$CH_3CH_2CH(NO_2)CH_3$ (2-nitrobutane)	-39.1	-260.9	-51.4	2.0	-2.8	-2.6	11.4	-5.7
191	$CH_3CH_2OCH_2CH_3$ (diethyl ether)	-60.3	-193.4	-20.4	16.0	6.6	18.6	23.9	14.5
192	CH_3-$CH(OCH_3)_2$ (1,1-dimethoxy ethane)	-93.1	-221.1	-21.8	20.7	14.9	23.6	29.9	19.2
193	$(CH_3)_3$C-SH (t-butanethiole)	-26.2	-181.5	-14.4	25.9	13.8	23.8	32.9	19.6
194	$(CH_3CH_2S)_2$ (diethyl disulfide)	-17.9	-201.3	-22.5	23.8	9.8	18.7	30.4	12.9
195	$(CH_3)_3$C-NH_2 (t-butylamine)	-28.9	-197.4	-18.2	20.3	13.0	22.2	30.0	21.2
196	$Si(CH_3)_4$ (tetramethyl silane)	-55.7	-175.6	-1.9	32.7	19.5	36.5	41.5	32.7
197	C_5H_6S (2-methyl thiopehene)	20.0	-198.1	-38.4	15.5	3.3	0.3	20.0	-6.0
198	C_5H7N (N-methyl pyrrole)	24.6	-217.2	-43.2	8.3	2.2	-1.7	15.6	-5.2
199	$C_5H_{10}O$ (tetrahydropyran)	-53.4	-227.8	-27.5	24.5	13.2	19.2	32.4	13.1
200	$C_2H_5COC_2H_5$ (diethyl ketone)	-61.6	-222.2	-30.3	16.7	6.3	13.7	25.3	9.9
201	$CH_3COOCH(CH_3)_2$ (isopropyl acetate)	-115.1	-255.3	-36.7	16.4	8.7	13.8	26.0	9.1
202	$C_5H_{10}S$ (tetrahydrothiopyran)	-15.2	-215.6	-24.5	30.1	14.9	20.5	36.8	13.9
203	$C_5H_{10}NH$ (piperidine)	-11.3	-233.3	-28.8	23.8	14.0	18.8	33.2	15.1
204	$(CH_3)_3COCH_3$ (t-butyl methyl ether)	-67.8	-233.0	-21.4	25.9	16.0	26.7	36.2	23.2
205	$C_6H_4F_2$ (1,3-difluuorobenzene)	-73.9	-249.4	-59.6	4.9	-1.1	-12.8	11.6	-18.3
206	$C_6H_4F_2$ (1,4-difluuorobenzene)	-73.3	-249.2	-59.5	4.9	-1.1	-12.8	11.6	-18.3
207	C_6H_5F (fluorobenzene)	-27.7	-227.1	-50.6	8.1	1.1	-7.6	14.7	-12.0
208	$(CH_3)_2CHOCH(CH_3)_2$ (diisopropyl ether)	-76.3	-272.6	-26.2	30.1	17.0	29.9	42.0	25.9
209	PF_5	-381.1	-123.4	-10.6	11.2	17.4	16.7	15.8	10.8
210	SF_6	-291.7	-171.6	-32.4	6.5	4.4	2.4	8.7	-8.1
211	P_4	14.1	-75.3	-19.5	5.0	-0.2	-5.0	3.2	-11.3
212	SO_3	-94.6	-110.4	-30.6	-6.3	-7.8	-10.8	-6.3	-18.2
213	SCl_2	-4.2	-47.4	-14.8	-0.4	-2.7	-6.1	-0.9	-9.6
214	$POCl_3$	-133.8	-88.5	-17.5	9.6	7.5	1.1	10.6	-3.9
215	PCl_5	-86.1	-97.9	-21.9	15.6	10.9	-0.9	16.3	-6.0
216	SO_2Cl_2	-84.8	-115.6	-31.5	0.8	-3.6	-9.7	0.7	-17.2
217	PCl_3	-69.0	-59.9	-14.7	3.9	2.9	-2.6	4.6	-5.5
218	S_2Cl_2	-4.0	-75.8	-27.5	-5.7	-8.7	-14.5	-6.2	-19.3

Table S1 – continued

219	$SiCl_2$ ($^1A_1$)	-40.3	-35.0	-5.9	4.9	4.6	1.7	5.8	0.1
220	CF_3Cl	-169.5	-115.8	-28.4	-0.0	-3.6	-6.3	1.1	-12.3
221	C_2F_6	-321.3	-203.3	-46.6	0.2	-1.9	-7.6	4.1	-15.6
222	CF_3	-111.3	-97.4	-28.6	-8.3	-9.7	-11.5	-7.1	-16.1
223	C_6H_5 (phenyl radical)	81.2	-199.1	-47.8	5.6	-1.5	-10.8	11.7	-13.6

Table S2: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	C	259.7	9.3	6.3	2.9	2.7	6.3	-0.3	2.9
2	S	238.9	3.6	0.4	0.2	-2.8	0.7	-3.4	-3.2
3	SH	238.9	4.0	-0.4	-1.8	-3.3	-0.5	-5.1	-4.0
4	Cl	299.1	5.2	0.2	-1.5	-2.5	-0.1	-4.9	-3.5
5	Cl_2	265.3	-1.6	-4.2	-6.3	-6.3	-4.0	-9.5	-7.5
6	OH	299.1	9.0	4.2	4.7	-0.8	4.3	-0.4	-1.7
7	O	313.9	9.1	10.2	12.5	1.2	11.7	5.4	2.3
8	O_2	278.9	10.1	7.0	7.9	5.4	7.2	3.7	3.2
9	P	241.9	2.2	0.4	-6.7	-3.1	0.3	-8.6	-1.6
10	PH	234.1	3.5	2.5	-3.6	-0.7	2.5	-5.9	0.2
11	PH_2	226.3	4.1	3.8	-1.4	0.4	3.9	-4.0	1.0
12	S_2	216.0	5.1	4.2	0.5	2.1	4.4	-2.3	1.3
13	Si	187.9	2.0	1.3	-4.5	-2.6	1.4	-6.6	-0.7

Table S3: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	C	29.1	12.0	7.0	1.6	0.9	6.4	-0.6	3.8
2	S	47.9	6.9	1.8	0.8	-2.1	1.5	-2.4	-2.4
3	SH	53.3	6.0	0.4	-1.6	-3.1	-0.2	-4.6	-3.7
4	Cl	83.4	7.8	1.7	-0.3	-1.3	1.1	-3.4	-2.3
5	Cl_2	55.6	9.7	12.2	14.0	9.7	13.8	9.3	7.2
6	OH	42.1	9.7	0.5	0.2	-3.6	-0.6	-3.4	-4.5
7	O	33.7	11.7	5.1	6.0	-1.2	4.6	1.3	-1.2
8	O_2	10.8	1.5	-0.3	2.3	-6.8	0.3	-3.2	-6.3
9	P	17.2	5.4	1.7	2.2	-1.9	1.7	-0.9	-2.3
10	PH	23.2	4.9	0.2	-0.5	-3.6	-0.1	-3.7	-4.1
11	PH_2	29.4	3.8	-1.4	-3.3	-5.0	-1.9	-6.2	-5.5
12	S_2	38.5	2.1	-0.1	-1.4	-4.0	0.1	-4.9	-4.1
13	Si	31.9	4.3	2.0	-4.3	-4.0	1.7	-5.9	0.1

Table S4: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	NH_3	211.9	-4.8	-1.3	-2.6	0.6	-0.5	-1.7	1.3
2	H_2O	171.8	-4.5	-2.0	-3.6	-0.4	-1.5	-2.4	0.7
3	HCCH	156.6	-2.4	2.6	1.3	5.2	3.8	2.3	5.0
4	SiH_4	156.5	-8.6	-0.9	0.9	2.4	1.3	0.6	0.4
5	PH_3	193.1	-9.0	-2.6	-1.7	0.7	-0.8	-1.7	-0.7
6	H_2S	173.7	-5.9	-0.2	-0.2	2.3	1.2	0.1	1.7
7	HCl	137.1	-5.6	-0.7	-1.2	1.4	0.5	-0.6	1.4
8	H_2	105.9	-4.3	-0.9	-2.7	0.3	-0.3	-1.8	1.1

Table S5: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	$(NH_3)_2$	3.15	3.32	1.08	0.08	-1.06	0.55	-1.22	-1.68
2	$(HF)_2$	4.57	3.13	0.73	0.07	-1.15	0.19	-1.33	-2.17
3	$(H_2O)_2$	4.97	4.46	1.56	0.60	-0.85	0.86	-0.81	-1.42
4	NH_3-H_2O	6.41	5.62	2.23	1.04	-0.73	1.37	-0.37	-0.82
5	$(HCONH_2)_2$	14.94	6.74	-0.20	-2.47	-6.25	-2.04	-4.74	-5.29
6	$(HCOOH)_2$	16.15	9.34	0.62	-1.93	-6.15	-1.73	-4.07	-4.32
7	C_2H_4-F2	1.06	3.93	2.30	1.84	0.88	2.02	0.26	-0.75
8	NH_3-F2	1.81	6.99	4.66	4.10	2.71	4.20	2.47	1.39
9	C_2H_2-ClF	3.81	6.33	2.31	0.72	-2.24	1.21	-1.03	-1.47
10	HCN-ClF	4.86	4.97	1.09	-0.05	-2.78	0.12	-1.79	-2.56
11	NH_3-Cl2	4.88	9.02	4.89	3.29	0.56	3.75	1.71	1.42
12	H_2O-ClF	5.36	7.10	2.98	1.63	-1.01	1.91	-0.10	-0.77
13	NH_3-ClF	10.62	14.81	8.09	5.69	2.08	6.18	3.99	4.17
14	$(H_2S)_2$	1.66	2.29	0.53	-0.60	-1.50	0.08	-1.68	-1.76
15	$(HCl)_2$	2.01	2.18	0.25	-0.75	-1.83	-0.22	-1.93	-2.23
16	HCl-H_2S	3.35	3.94	1.29	-0.09	-1.52	0.59	-1.29	-1.33
17	CH_3Cl-HCl	3.55	3.13	0.02	-1.44	-3.37	-0.77	-3.07	-3.46
18	HCN-CH_3SH	3.59	2.49	0.12	-1.18	-2.46	-0.47	-2.63	-2.96
19	CH_3SH-HCl	4.16	5.83	2.00	0.04	-2.01	0.95	-1.50	-1.44
20	HeNe	0.04	0.32	0.28	0.14	0.37	0.30	-0.26	-0.41
21	HeAr	0.06	0.48	0.40	0.23	0.47	0.42	-0.25	-0.44
22	Ne_2	0.08	0.18	0.15	-0.09	0.21	0.18	-0.65	-0.82
23	NeAr	0.13	0.20	0.06	-0.25	-0.02	0.07	-0.89	-1.09
24	CH_4-Ne	0.22	0.22	0.08	-0.29	-0.02	0.10	-1.03	-1.25
25	C_6H_6-Ne	0.47	0.52	-0.08	-0.81	-0.65	-0.15	-2.17	-2.69
26	$(CH_4)_2$	0.51	0.47	-0.50	-1.33	-1.69	-0.67	-2.57	-2.96
27	$(C_2H_2)_2$	1.34	0.84	-0.24	-1.11	-1.57	-0.46	-2.28	-2.61
28	$(C_2H_4)_2$	1.42	1.20	-0.91	-2.27	-3.43	-1.36	-4.09	-4.71
29	Sandwich C_6H_6	1.81	-1.10	-3.80	-5.86	-6.69	-4.36	-8.28	-8.66
30	T-Shaped C_6H_6	2.74	0.13	-2.97	-4.88	-5.79	-3.68	-6.93	-7.06
31	Parallel C_6H_6	2.78	-0.69	-4.30	-6.77	-8.26	-5.14	-9.39	-9.67

Table S6: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	$H + HCl \rightarrow H_2 + Cl$	5.7	-8.9	-5.2	-8.2	-6.3	-4.7	-7.1	-3.7
2	$OH + H_2 \rightarrow H + H_2O$	5.7	-23.4	-11.5	-8.7	-6.3	-8.5	-7.9	-8.3
3	$CH_3 + H_2 \rightarrow H + CH_4$	12.1	-17.4	-8.2	-4.9	-3.6	-5.7	-4.3	-5.4
4	$OH + CH_4 \rightarrow CH_3 + H_2O$	6.7	-23.3	-11.8	-9.0	-6.5	-8.9	-8.0	-8.4
5	$H + H_2 \rightarrow H_2 + H$	9.6	-12.4	-5.9	-6.7	-6.2	-4.5	-6.7	-5.3
6	$OH + NH_3 \rightarrow H_2O + NH_2$	3.2	-27.2	-15.3	-12.7	-9.7	-12.3	-11.6	-11.6
7	$HCl + CH_3 \rightarrow Cl + CH_4$	1.7	-15.1	-7.5	-5.1	-2.8	-5.4	-3.9	-4.2
8	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	3.4	-23.7	-11.9	-9.0	-6.5	-8.9	-8.0	-8.3
9	$F + H_2 \rightarrow HF + H$	1.8	-24.7	-13.7	-12.4	-8.9	-11.2	-11.1	-10.0
10	$O + CH_4 \rightarrow OH + CH_3$	13.7	-23.2	-13.5	-11.3	-7.3	-10.9	-9.8	-9.6
11	$H + PH_3 \rightarrow PH_2 + H_2$	3.1	-10.5	-4.8	-5.7	-5.0	-3.7	-5.4	-3.9
12	$H + HO \rightarrow H_2 + O$	10.7	-12.8	-7.3	-9.5	-9.4	-6.3	-9.3	-6.7
13	$H + H_2S \rightarrow H_2 + HS$	3.5	-10.3	-4.7	-5.7	-4.7	-3.5	-5.3	-3.6
14	$O + HCl \rightarrow OH + Cl$	9.8	-32.6	-20.2	-18.6	-13.9	-17.3	-16.9	-15.7
15	$NH_2 + CH_3 \rightarrow CH_4 + NH$	8.0	-16.7	-7.6	-4.9	-4.1	-5.3	-4.2	-4.9
16	$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$	7.5	-13.6	-4.9	-2.0	-1.2	-2.6	-1.2	-2.0
17	$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$	10.4	-20.0	-8.9	-5.2	-3.5	-5.9	-4.3	-5.4
18	$NH_2 + CH_4 \rightarrow CH_3 + NH_3$	14.5	-20.6	-10.1	-6.5	-4.9	-7.3	-5.8	-6.9
19	$C_5H_8 \rightarrow C_5H_8$	38.4	-13.4	-7.2	-2.6	-3.3	-5.0	-3.7	-7.6

Table S7: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	$H + HCl \rightarrow H_2 + Cl$	8.7	-19.0	-9.8	-6.0	-5.0	-7.2	-5.4	-7.1
2	$OH + H_2 \rightarrow H + H_2O$	21.2	-10.4	-8.0	-11.4	-8.9	-7.9	-10.3	-6.6
3	$CH_3 + H_2 \rightarrow H + CH_4$	15.3	-10.4	-5.9	-7.6	-6.8	-5.1	-7.2	-5.2
4	$OH + CH_4 \rightarrow CH_3 + H_2O$	19.6	-17.8	-11.2	-9.6	-6.6	-9.5	-8.2	-7.5
5	$H + H_2 \rightarrow H_2 + H$	9.6	-12.4	-5.9	-6.7	-6.2	-4.5	-6.7	-5.3
6	$OH + NH_3 \rightarrow H_2O + NH_2$	12.7	-24.2	-14.2	-11.8	-8.6	-11.6	-10.5	-10.3
7	$HCl + CH_3 \rightarrow Cl + CH_4$	7.9	-18.2	-9.7	-5.5	-4.6	-7.3	-5.1	-7.4
8	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	19.9	-15.5	-9.6	-8.2	-4.9	-8.1	-6.5	-5.7
9	$F + H_2 \rightarrow HF + H$	33.4	-8.5	-9.1	-13.7	-10.5	-9.9	-12.1	-7.4
10	$O + CH_4 \rightarrow OH + CH_3$	8.1	-17.6	-8.9	-6.8	-5.8	-6.8	-6.0	-6.0
11	$H + PH_3 \rightarrow PH_2 + H_2$	23.2	-13.5	-4.9	-1.3	0.8	-2.5	-0.7	-2.2
12	$H + HO \rightarrow H_2 + O$	13.1	-25.4	-14.1	-11.3	-7.7	-11.1	-10.2	-10.4
13	$H + H_2S \rightarrow H_2 + HS$	17.3	-17.7	-7.8	-2.9	-1.9	-4.9	-2.7	-5.3
14	$O + HCl \rightarrow OH + Cl$	10.4	-30.1	-18.0	-14.5	-14.2	-14.9	-14.3	-15.3
15	$NH_2 + CH_3 \rightarrow CH_4 + NH$	22.4	-19.8	-11.5	-8.8	-5.8	-9.2	-7.5	-7.8
16	$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$	18.3	-19.5	-10.5	-7.4	-4.5	-8.0	-6.1	-6.5
17	$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$	17.4	-14.7	-7.7	-5.1	-3.0	-5.8	-3.9	-4.2
18	$NH_2 + CH_4 \rightarrow CH_3 + NH_3$	17.8	-18.0	-10.5	-7.9	-5.9	-8.4	-6.8	-7.1
19	$C_5H_8 \rightarrow C_5H_8$	38.4	-13.4	-7.2	-2.6	-3.3	-5.0	-3.7	-7.6

Table S8: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	$H + N_2O \rightarrow OH + N_2$	18.14	-15.03	-7.66	-9.11	-6.66	-6.13	-8.23	-5.53
2	$H + FH \rightarrow HF + H$	42.18	-22.91	-14.24	-15.45	-12.47	-12.28	-14.58	-11.65
3	$H + ClH \rightarrow + HCl\ H$	18.00	-15.84	-8.31	-8.18	-7.62	-6.53	-7.99	-7.09
4	$H + FCH_3 \rightarrow HF + CH_3$	30.38	-16.36	-11.13	-13.53	-9.67	-10.17	-12.23	-8.60
5	$H + F_2 \rightarrow HF + F$	2.27	28.92	35.65	32.74	34.40	36.73	33.86	38.23
6	$CH_3 + FCl \rightarrow CH_3F + Cl$	7.43	-17.97	-12.96	-13.62	-8.38	-11.90	-11.09	-7.97
7	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-17.84	-14.16	-14.05	-8.07	-13.14	-11.04	-8.45
8	$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	13.38	-8.19	-7.75	-8.28	-5.28	-7.47	-7.79	-7.13
9	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.10	-12.54	-9.68	-10.10	-3.76	-8.83	-7.40	-4.97
10	$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	13.61	-7.79	-7.43	-8.90	-4.66	-7.18	-8.13	-6.65
11	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	-12.54	-17.70	-14.10	-14.23	-8.54	-13.05	-11.51	-8.94
12	$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	2.89	-5.53	-5.30	-6.29	-3.69	-5.12	-5.93	-5.03
13	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	-2.78	-18.18	-14.35	-13.80	-8.26	-13.30	-10.82	-8.66
14	$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	10.96	-10.97	-10.56	-10.70	-8.14	-10.26	-10.23	-9.89
15	$H + N_2 \rightarrow HN_2$	14.69	-16.87	-9.38	-9.33	-9.05	-7.69	-9.16	-8.35
16	$H + CO \rightarrow HCO$	3.17	-10.91	-4.90	-5.15	-4.48	-3.65	-4.89	-3.89
17	$H + C2H_4 \rightarrow CH_3CH_2$	1.72	-7.14	-1.83	-2.40	-1.43	-0.77	-1.99	-0.70
18	$CH_3 + C2H_4 \rightarrow CH_3CH_2CH_2$	6.85	-12.50	-5.28	-2.12	0.16	-3.26	-0.74	-1.55
19	$HCN \rightarrow HNC$	48.16	-3.24	-2.46	-1.30	-2.27	-2.02	-1.98	-2.96

Table S9: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	$H + N_2O \rightarrow OH + N_2$	83.22	-51.21	-30.94	-21.92	-23.65	-25.45	-22.78	-27.84
2	$H + FH \rightarrow HF + H$	42.18	-22.91	-14.24	-15.45	-12.47	-12.28	-14.58	-11.65
3	$H + ClH \rightarrow HCl + H$	18.00	-15.84	-8.31	-8.18	-7.62	-6.53	-7.99	-7.09
4	$H + FCH_3 \rightarrow HF + CH_3$	57.02	-24.98	-15.83	-14.74	-8.93	-13.42	-12.66	-10.65
5	$H + F_2 \rightarrow HF + F$	106.18	7.82	19.56	19.71	25.41	22.31	21.38	24.69
6	$CH_3 + FCl \rightarrow CH_3F + Cl$	60.17	-22.45	-18.67	-18.58	-12.84	-17.71	-16.38	-14.24
7	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.34	-17.84	-14.16	-14.05	-8.07	-13.14	-11.04	-8.45
8	$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	13.38	-8.19	-7.75	-8.28	-5.28	-7.47	-7.79	-7.13
9	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	3.10	-12.54	-9.68	-10.10	-3.76	-8.83	-7.40	-4.97
10	$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	13.61	-7.79	-7.43	-8.90	-4.66	-7.18	-8.13	-6.65
11	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	20.11	-10.55	-8.19	-7.71	-2.07	-7.53	-4.90	-3.06
12	$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	29.62	-6.89	-6.89	-7.32	-3.72	-6.75	-6.52	-5.80
13	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	17.33	-17.35	-14.21	-14.56	-8.14	-13.28	-11.48	-8.49
14	$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	47.20	1.48	-2.86	-5.67	-1.26	-3.95	-4.43	-1.77
15	$H + N_2 \rightarrow HN_2$	10.72	-1.57	-1.93	-2.54	-0.94	-2.00	-2.52	-1.86
16	$H + CO \rightarrow HCO$	22.68	3.38	1.73	0.41	2.49	1.33	0.48	1.75
17	$H + C_2H_4 \rightarrow CH_3CH_2$	41.75	-2.35	-1.41	-3.47	-0.20	-1.33	-3.14	-0.61
18	$CH_3 + C_2H_4 \rightarrow CH_3CH_2CH_2$	32.97	0.24	-3.05	-7.85	-3.47	-4.25	-6.79	-2.40
19	$HCN \rightarrow HNC$	33.11	-2.24	-2.38	-1.22	-1.94	-2.24	-1.71	-2.68

Table S10: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	H_2	0.741	0.025	0.010	0.006	0.004	0.006	0.010	0.012
2	Li_2	2.673	0.045	0.065	0.047	0.094	0.066	0.079	0.120
3	LiH	1.595	0.011	0.012	0.005	0.019	0.011	0.014	0.024
4	LiF	1.564	-0.010	0.012	0.013	0.015	0.017	0.019	0.022
5	LiCl	2.021	-0.016	0.004	0.009	0.007	0.008	0.017	0.019
6	LiO	1.688	-0.011	0.011	0.013	0.018	0.016	0.019	0.022
7	Be2	2.440	-0.030	0.001	0.012	0.040	0.012	0.036	0.045
8	BeH	1.343	0.024	0.019	0.008	0.021	0.016	0.016	0.026
9	BeF	1.361	0.004	0.019	0.021	0.021	0.022	0.024	0.025
10	BeO	1.331	0.002	0.015	0.015	0.016	0.017	0.017	0.017
11	BeS	1.742	0.002	0.015	0.018	0.015	0.017	0.020	0.017
12	B_2	1.590	0.016	0.029	0.029	0.034	0.031	0.035	0.038
13	BH	1.232	0.025	0.020	0.009	0.020	0.017	0.018	0.029
14	BF	1.263	-0.002	0.013	0.014	0.016	0.016	0.017	0.018
15	BF_3	1.313	-0.002	0.012	0.016	0.012	0.016	0.017	0.014
16	BCl	1.715	-0.005	0.016	0.021	0.021	0.021	0.025	0.024
17	BCl_3	1.742	-0.012	0.006	0.017	0.007	0.011	0.017	0.008
18	BN	1.281	0.042	0.051	0.053	0.055	0.053	0.055	0.053
19	BO	1.204	0.001	0.010	0.011	0.010	0.012	0.012	0.012
20	BS	1.609	0.000	0.012	0.015	0.012	0.014	0.016	0.014
21	C_2	1.242	0.151	0.162	0.158	0.165	0.164	0.163	0.167
22	CH	1.120	0.021	0.017	0.013	0.015	0.015	0.018	0.022
23	CH_4	1.087	0.010	0.009	0.008	0.006	0.008	0.011	0.011
24	CF	1.272	-0.006	0.015	0.022	0.015	0.020	0.022	0.016
25	CF_4	1.323	-0.003	0.015	0.022	0.012	0.019	0.021	0.015
26	CCl	1.645	-0.010	0.015	0.030	0.015	0.021	0.028	0.017
27	CCl_4	1.767	-0.009	0.015	0.035	0.014	0.022	0.032	0.014
28	CN	1.172	-0.006	0.002	0.003	0.002	0.004	0.004	0.004
29	CO	1.128	-0.000	0.008	0.009	0.008	0.010	0.010	0.010
30	CO^+	1.115	-0.000	0.007	0.008	0.006	0.009	0.009	0.008
31	CO_2	1.160	0.003	0.011	0.013	0.010	0.013	0.014	0.012
32	CP	1.562	-0.007	0.005	0.008	0.004	0.007	0.009	0.006
33	CS	1.535	-0.002	0.011	0.013	0.011	0.014	0.015	0.013
34	CS_2	1.553	-0.003	0.009	0.014	0.007	0.012	0.014	0.009
35	N_2	1.098	-0.003	0.005	0.005	0.004	0.006	0.006	0.006
36	N_2^+	1.116	-0.010	-0.002	-0.000	-0.002	-0.000	0.001	-0.001
37	NH	1.036	0.019	0.015	0.016	0.013	0.013	0.018	0.017
38	NH^+	1.070	0.030	0.021	0.021	0.016	0.019	0.024	0.023
39	NF	1.317	-0.013	0.010	0.026	0.008	0.017	0.022	0.009
40	NCl	1.611	-0.019	0.007	0.027	0.007	0.014	0.024	0.008
41	NO	1.151	-0.004	0.007	0.011	0.005	0.009	0.011	0.007
42	NO^+	1.063	-0.001	0.007	0.008	0.006	0.008	0.009	0.007
43	NS	1.494	-0.002	0.012	0.017	0.010	0.016	0.017	0.012
44	O_2	1.208	-0.004	0.011	0.021	0.007	0.014	0.019	0.009
45	O_2^+	1.116	-0.005	0.006	0.012	0.003	0.008	0.011	0.005
46	OH	0.970	0.016	0.013	0.015	0.008	0.013	0.017	0.014
47	OH^+	1.029	0.027	0.019	0.022	0.014	0.017	0.023	0.019
48	OF	1.358	-0.026	0.001	0.021	-0.005	0.009	0.015	-0.003
49	F_2	1.412	-0.027	0.002	0.021	-0.006	0.010	0.014	-0.004
50	F_2^+	1.322	-0.030	-0.006	0.012	-0.014	0.001	0.006	-0.011
51	HF	0.917	0.014	0.013	0.016	0.007	0.013	0.016	0.013

Table S10 – continued

52	HF^+	1.001	0.028	0.022	0.027	0.014	0.021	0.026	0.019
53	Na_2	3.079	-0.070	0.000	-0.000	0.106	0.029	0.038	0.109
54	NaH	1.887	-0.015	0.006	0.000	0.026	0.011	0.014	0.030
55	NaF	1.926	-0.022	0.016	0.020	0.033	0.026	0.025	0.028
56	NaCl	2.361	-0.031	0.009	0.019	0.027	0.019	0.027	0.028
57	NaO	2.052	-0.021	0.020	0.025	0.043	0.031	0.032	0.033
58	MgH	1.730	0.023	0.027	0.026	0.034	0.028	0.031	0.030
59	MgF	1.750	0.006	0.032	0.037	0.039	0.039	0.038	0.035
60	MgCl	2.196	0.002	0.029	0.042	0.038	0.037	0.043	0.033
61	MgO	1.748	-0.022	0.002	0.008	0.005	0.009	0.009	0.004
62	Al_2	2.466	-0.005	0.023	0.053	0.034	0.031	0.052	0.027
63	AlH	1.648	0.031	0.032	0.026	0.029	0.031	0.032	0.037
64	AlF	1.654	0.005	0.028	0.034	0.030	0.034	0.035	0.030
65	AlCl	2.130	0.006	0.032	0.048	0.034	0.039	0.046	0.033
66	AlO	1.618	-0.005	0.014	0.021	0.013	0.019	0.020	0.013
67	AlS	2.029	0.000	0.020	0.034	0.017	0.025	0.031	0.017
68	Si_2	2.246	-0.096	0.040	-0.063	0.039	0.045	0.053	0.041
69	SiH	1.520	0.025	0.025	0.021	0.021	0.025	0.026	0.029
70	SiH_4	1.480	0.013	0.013	0.007	0.012	0.013	0.012	0.017
71	SiF	1.601	0.010	0.032	0.038	0.031	0.037	0.037	0.032
72	SiF_4	1.553	0.008	0.028	0.032	0.027	0.033	0.032	0.028
73	SiCl	2.058	0.002	0.027	0.046	0.026	0.034	0.042	0.025
74	SiCl	2.019	-0.003	0.021	0.035	0.021	0.027	0.034	0.021
75	SiN	1.572	-0.008	0.007	0.010	0.006	0.011	0.011	0.008
76	SiO	1.510	0.005	0.019	0.021	0.017	0.022	0.022	0.019
77	SiS	1.929	0.006	0.022	0.030	0.019	0.026	0.029	0.021
78	P_2	1.893	-0.001	0.013	0.019	0.009	0.016	0.018	0.012
79	P_4	2.210	-0.022	-0.001	0.022	-0.010	0.004	0.016	-0.004
80	PH	1.421	0.021	0.020	0.018	0.015	0.019	0.022	0.022
81	PF	1.589	0.007	0.029	0.039	0.027	0.036	0.037	0.028
82	PCl	2.015	-0.008	0.017	0.040	0.013	0.024	0.034	0.014
83	PN	1.491	-0.004	0.008	0.010	0.006	0.011	0.011	0.009
84	PO	1.476	0.007	0.021	0.025	0.018	0.024	0.024	0.020
85	S_2	1.889	0.007	0.022	0.040	0.017	0.027	0.036	0.019
86	SH	1.341	0.018	0.016	0.016	0.010	0.015	0.019	0.017
87	SF	1.601	-0.003	0.022	0.037	0.016	0.029	0.032	0.018
88	SF_6	1.561	0.009	0.036	0.049	0.031	0.043	0.046	0.033
89	SO	1.481	0.009	0.024	0.034	0.021	0.028	0.032	0.023
90	SO_3	1.420	0.009	0.024	0.030	0.019	0.028	0.029	0.023
91	Cl_2	1.988	-0.007	0.017	0.052	0.009	0.026	0.043	0.012
92	Cl_2^+	1.891	0.003	0.023	0.051	0.015	0.029	0.043	0.018
93	HCl	1.275	0.016	0.014	0.016	0.007	0.013	0.017	0.014
94	HCl^+	1.315	0.025	0.018	0.020	0.011	0.017	0.022	0.018
95	ClF	1.628	-0.004	0.023	0.045	0.016	0.032	0.039	0.018
96	ClO	1.570	-0.015	0.013	0.034	0.006	0.021	0.028	0.009

Table S11: 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		LDA	PBE	BLYP	OLYP	PBE-LS	CAP-LYP	CAP-PBE
1	H_2	4401.2	-218.6	-85.8	-55.7	-23.5	-48.9	-91.8	-102.4
2	Li_2	351.4	-17.8	-21.3	-22.3	-29.6	-21.4	-29.5	-33.5
3	LiH	1405.7	-29.9	-28.5	-19.1	-38.4	-25.4	-38.5	-56.2
4	LiF	910.6	13.8	-16.4	-17.4	-29.1	-22.7	-29.3	-39.1
5	LiCl	643.0	10.6	-3.6	-10.3	-7.3	-6.6	-17.2	-19.0
6	LiO	814.6	3.7	-18.5	-20.6	-33.8	-25.0	-29.9	-35.0
7	LiNa	256.8	-4.4	-11.1	-13.6	-20.5	-12.2	-19.3	-21.5
8	Be_2	267.9	99.9	78.7	53.3	57.6	73.1	46.2	62.5
9	BeH	2060.8	-103.7	-86.3	-63.6	-93.5	-80.6	-83.8	-99.8
10	BeH^+	2221.7	-137.9	-112.5	-100.3	-117.1	-105.1	-112.8	-103.1
11	BeF	1247.4	-5.6	-41.2	-48.1	-48.4	-48.7	-56.0	-56.8
12	BeCl	846.7	-16.4	-32.7	-45.6	-44.1	-36.7	-48.8	-41.1
13	BeO	1487.3	7.6	-33.2	-39.6	-37.9	-42.5	-43.5	-36.0
14	BeS	997.9	-0.6	-20.4	-35.7	-20.8	-25.1	-36.4	-23.1
15	B_2	1051.3	-15.1	-39.1	-58.7	-51.5	-44.4	-64.8	-53.9
16	BH	2366.9	-138.0	-124.4	-89.5	-122.7	-115.8	-123.3	-158.4
17	BF	1402.1	4.7	-51.0	-57.1	-59.5	-63.3	-64.7	-66.6
18	BCl	840.3	-2.7	-31.0	-48.8	-34.3	-37.9	-50.5	-38.6
19	BN	1514.6	30.4	1.4	-19.5	-18.7	-6.6	-25.0	-4.3
20	BO	1885.7	2.9	-38.5	-49.9	-38.9	-48.2	-52.4	-42.2
21	BS	1180.2	2.9	-18.5	-38.5	-19.0	-24.0	-37.5	-19.5
22	C_2	1854.7	45.2	2.2	-23.1	4.4	-7.1	-24.6	-5.9
23	CH	2858.5	-117.8	-127.1	-132.4	-115.6	-121.7	-153.5	-148.1
24	CF	1308.1	24.4	-54.2	-90.8	-55.0	-72.8	-85.1	-54.8
25	CN	2068.6	73.0	25.3	5.7	27.9	14.9	4.0	20.0
26	CO	2169.8	11.7	-40.2	-53.5	-38.6	-51.5	-56.5	-45.5
27	CO^+	2214.2	37.7	-10.6	-38.4	-4.0	-22.6	-36.6	-10.1
28	CP	1239.7	38.2	9.6	-10.7	9.9	2.4	-9.4	8.6
29	CS	1285.2	5.7	-22.9	-41.2	-19.6	-29.8	-40.3	-24.2
30	N_2	2358.6	43.7	-5.5	-22.7	1.5	-15.9	-24.0	-7.7
31	N_2^+	2207.0	114.4	58.8	27.8	65.4	45.2	30.7	55.7
32	NH	3282.3	-133.3	-109.1	-146.7	-102.6	-104.9	-159.1	-133.7
33	NF	1141.4	52.9	-9.4	-63.6	5.2	-28.6	-51.5	18.9
34	NCl	828.0	53.4	8.8	-38.5	7.5	-4.5	-29.0	10.1
35	NO	1904.2	56.0	-11.8	-54.2	0.3	-27.2	-45.7	0.8
36	NO^+	2376.4	42.2	-13.7	-40.5	-2.7	-26.5	-37.9	-12.7
37	NS	1218.7	44.1	8.1	-21.9	14.2	-1.7	-16.0	11.7
38	O_2	1580.2	42.7	-21.9	-85.3	-1.3	-40.6	-67.1	-5.7
39	O_2^+	1904.8	98.9	32.3	-30.1	49.3	10.5	-14.2	44.3
40	OH	3737.8	-143.0	-131.6	-175.2	-89.8	-134.0	-175.9	-127.9
41	OH^+	3113.4	-211.4	-157.5	-200.5	-133.4	-148.7	-202.4	-146.9
42	F_2	916.6	144.8	78.2	42.1	81.1	57.2	53.7	89.6
43	F_2^+	1073.3	142.2	76.5	30.2	88.9	54.4	46.2	91.5
44	HF	4138.3	-148.7	-158.6	-207.4	-93.0	-163.8	-200.5	-144.1
45	HF^+	3090.5	-222.4	-178.4	-229.3	-127.5	-175.7	-216.2	-144.9
46	Na2	159.1	3.8	-0.7	-6.0	-11.8	-3.9	-8.6	-10.5
47	NaH	1172.2	-3.7	-23.7	-18.3	-59.2	-27.6	-39.2	-55.9
48	NaF	535.7	15.9	-16.5	-18.2	-35.9	-24.1	-24.5	-31.2
49	NaO	492.3	0.8	-24.1	-28.4	-44.8	-30.8	-34.9	-35.7
50	MgH	1495.2	-92.0	-88.3	-103.7	-100.4	-88.9	-104.2	-77.1
51	MgH^+	1699.1	-51.1	-46.4	-46.5	-59.7	-46.9	-54.0	-39.3

Table S11 – continued

52	MgO	784.8	57.4	19.9	9.5	11.4	9.2	8.4	17.1
53	MgS	528.7	15.5	-1.6	-17.6	-5.0	-6.9	-15.7	-0.8
54	Al_2	350.0	13.0	-8.2	-21.0	3.0	-11.6	-16.8	-7.3
55	AlH	1682.6	-103.1	-100.2	-99.4	-86.8	-99.0	-111.2	-108.9
56	AlF	802.3	-18.8	-50.5	-59.2	-55.0	-58.7	-60.8	-54.2
57	AlCl	481.3	-7.1	-22.5	-37.6	-22.1	-27.6	-35.6	-22.3
58	AlO	979.2	25.6	-19.1	-39.2	-20.0	-31.8	-35.2	-14.9
59	AlS	617.1	2.5	-15.7	-40.1	-11.6	-21.6	-34.0	-9.2
60	Si_2	511.0	39.7	-26.2	-0.1	-24.1	-29.0	-41.3	-24.0
61	SiH	2041.8	-79.5	-92.8	-89.2	-78.3	-93.9	-110.0	-97.2
62	SiH^+	2157.2	-133.8	-114.2	-107.7	-101.0	-108.5	-120.9	-120.3
63	SiF	857.2	-9.1	-45.4	-59.7	-52.7	-60.8	-57.5	-49.8
64	SiCl	535.6	6.5	-13.0	-35.9	-13.5	-31.4	-30.9	-9.9
65	SiN	1151.4	34.3	-1.6	-17.0	-2.6	-10.8	-15.4	-1.4
66	SiO	1241.5	-12.3	-46.9	-56.5	-43.4	-55.8	-55.6	-45.5
67	SiS	749.6	-9.4	-24.2	-41.4	-20.0	-29.0	-38.1	-21.8
68	P_2	780.8	15.8	1.4	-16.7	7.6	-2.7	-13.1	4.1
69	P_2^+	672.2	12.5	2.4	-25.6	6.2	-1.8	-20.9	5.3
70	PH	2365.2	-85.2	-78.5	-104.2	-58.5	-78.1	-108.4	-80.9
71	PF	846.8	0.7	-37.9	-61.0	-36.1	-49.4	-54.8	-33.4
72	PCl	551.4	11.4	-19.2	-44.9	-17.2	-26.1	-39.4	-5.9
73	PN	1337.2	34.9	2.3	-12.1	9.4	-5.9	-10.5	4.2
74	PO	1233.3	8.2	-27.3	-46.4	-20.2	-37.2	-42.4	-22.9
75	S_2	725.6	-5.7	-19.4	-54.9	-14.3	-25.2	-45.9	-14.4
76	SO	1149.2	-2.2	-40.0	-77.4	-32.4	-51.7	-67.8	-32.3
77	Cl_2	559.7	8.1	-16.7	-53.7	-12.8	-25.7	-43.8	-9.5
78	Cl_2^+	645.6	3.5	-20.6	-66.3	-17.3	-32.0	-55.1	-15.2
79	HCl	2990.9	-101.6	-91.1	-135.8	-47.7	-89.8	-132.6	-87.5
80	HCl+	2673.7	-139.7	-113.4	-148.9	-79.0	-107.2	-147.2	-106.4
81	ClF	786.1	22.3	-22.7	-59.8	-16.7	-37.1	-49.2	-13.7
82	ClO	853.8	64.3	9.5	-39.8	17.4	-8.1	-25.3	19.1

$$\text{Lieb} - \text{Oxford ratio} = \frac{E_x[\rho]}{\int \rho^{4/3}(\mathbf{r})\, d\mathbf{r}} \geq -1.679 \tag{S1}$$

Table S12: Calculated Lieb-Oxford ratios for all test sets.

	Molecule	CAP-PBE
	G3/99	
1	LiH	-0.8367
2	BeH	-1.0462
3	CH	-1.0304
4	$CH_2(^3B_1)$	-1.0252
5	$CH_2(^1A_1)$	-0.8154
6	CH_3	-1.0232
7	CH_4	-0.8100
8	NH	-1.0215
9	NH_2	-1.0192
10	NH_3	-0.8063
11	OH	-1.0155
12	H_2O	-0.8034

Table S12 – continued

13	FH	-0.8010
14	$SiH_2(^1A_1)$	-0.7926
15	$SiH_2(^3B_1)$	-0.9984
16	SiH_3	-0.9987
17	SiH_4	-0.7929
18	PH_2	-0.9964
19	PH_3	-0.7908
20	H_2S	-0.7892
21	HCl	-0.7879
22	Li_2	-0.8362
23	LiF	-0.8049
24	HCCH	-0.8096
25	CH_2CH_2	-0.8088
26	CH_3CH_3	-0.8081
27	CN	-1.0196
28	HCN	-0.8081
29	CO	-0.8063
30	CHO	-1.0154
31	CH_2O	-0.8055
32	CH_3OH	-0.8047
33	N_2	-0.8068
34	N_2H_4	-0.8048
35	NO	-1.0143
36	O_2	-1.0122
37	H_2O_2	-0.8028
38	F_2	-0.8008
39	CO_2	-0.8036
40	Na_2	-0.7965
41	Si_2	-0.9971
42	P_2	-0.7896
43	S_2	-0.9934
44	Cl_2	-0.7874
45	NaCl	-0.7905
46	SiO	-0.7945
47	CS	-0.7924
48	SO	-0.9979
49	ClO	-0.9967
50	ClF	-0.7908
51	Si_2H_6	-0.7920
52	CH_3Cl	-0.7911
53	CH_3SH	-0.7923
54	HOCl	-0.7910
55	SO_2	-0.7935
56	BF_3	-0.8008
57	BCl_3	-0.7882
58	AlF_3	-0.7968
59	$AlCl_3$	-0.7881
60	CF_4	-0.7997
61	CCl4	-0.7878
62	COS	-0.7938
63	CS_2	-0.7901
64	COF_2	-0.8010
65	SiF_4	-0.7962
66	SiCl4	-0.7875
67	N_2O	-0.8039
68	NOCl	-0.7931

Table S12 – continued

69	NF_3	-0.8004
70	PF_3	-0.7948
71	O_3	-0.8026
72	F_2O	-0.8010
73	ClF_3	-0.7935
74	CF_2CF_2	-0.8005
75	CCl_2CCl_2	-0.7886
76	CF_3CN	-0.8016
77	CH_3CCH(propyne)	-0.8082
78	CH_2CCH_2(allene)	-0.8081
79	$C3H_4$(cyclopropene)	-0.8075
80	CH_3CHCH_2(propylene)	-0.8077
81	$C3H_6$(cyclopropane)	-0.8068
82	$C3H_8$(propane)	-0.8072
83	C_4H_6(1,3-butadien)	-0.8075
84	C_4H_6(2-butyne)	-0.8075
85	C_4H_6(methylene cyclopropane)	-0.8069
86	C_4H_6(bicyclobutane)	-0.8062
87	C_4H_6(cyclobutene)	-0.8067
88	C_4H_8(cyclobutane)	-0.8064
89	C_4H_8(isobutene)	-0.8070
90	C_4H_{10}(butane)	-0.8068
91	C_4H_{10}(isobutane)	-0.8067
92	C_5H_8(spiropentane)	-0.8061
93	C_6H_6(benzene)	-0.8062
94	CH_2F_2	-0.8012
95	CHF_3	-0.8003
96	CH_2Cl_2	-0.7891
97	$CHCl_3$	-0.7883
98	CH_3NH_2(methylamine)	-0.8062
99	CH_3CN(acetronitrile)	-0.8072
100	CH_3NO_2(nitromethane)	-0.8032
101	CH_3ONO(methyl nitrite)	-0.8035
102	CH_3SiH_3(methyl silane)	-0.7956
103	HCOOH(formic acid)	-0.8032
104	$HCOOCH_3$(methyl formate)	-0.8038
105	CH_3CONH_2(acetamide)	-0.8043
106	C_2H_4NH(aziridine)	-0.8058
107	C_2N_2(cyanogen)	-0.8070
108	$(CH_3)_2NH$(dimethylamine)	-0.8060
109	$CH_3CH_2NH_2$(ethylamine)	-0.8060
110	CH_2CO(ketene)	-0.8055
111	C_2H_4O(oxirane)	-0.8049
112	CH_3CHO(acetaldehyde)	-0.8054
113	HCOCHO(glyoxal)	-0.8044
114	CH_3CH_2OH(ethanol)	-0.8049
115	CH_3OCH_3(dimethyl ether)	-0.8050
116	C_2H_4S(thiirane)	-0.7940
117	$(CH_3)_2SO$(dimethyl sulfoxide)	-0.7954
118	C_2H_5SH(ethanethiol)	-0.7944
119	CH_3SCH_3(dimethyl sulfide)	-0.7944
120	CH_2CHF(vinil fluoride)	-0.8039
121	C_2H_5Cl(ethyl chloride)	-0.7932
122	CH_2CHCl(vinyl chloride)	-0.7931
123	CH_2CHCN(acrylonitrile)	-0.8072
124	CH_3COCH_3(acetone)	-0.8054

Table S12 – continued

125	CH_3COOH(acetic acid)	-0.8036
126	CH_3COF(acetyl fluoride)	-0.8029
127	CH_3COCl(acetyl chloride)	-0.7944
128	$CH_3CH_2CH_2Cl$(propyl chloride)	-0.7948
129	$(CH_3)_2CHOH$(isopropanol)	-0.8049
130	$C_2H_5OCH_3$(methyl ethyl ether)	-0.8051
131	$(CH_3)_3N$(trimethylamine)	-0.8058
132	C_4H_4O(furan)	-0.8047
133	C_4H_4S(thiophene)	-0.7964
134	C_4H_5N(pyrrole)	-0.8053
135	C_5H_5N(pyridine)	-0.8057
136	H_2	-0.8433
137	SH	-0.9945
138	CCH(^2A',C_s)	-1.0215
139	$CHCH_2$(^2A',C_s)	-1.0201
140	CH_3CO(^2A',C_s)	-1.0153
141	CH_2OH(^2A,C_1)	-1.0144
142	CH_3O(^2A',C_s)	-1.0152
143	CH_3CH_2O(^2A",C_s)	-1.0151
144	CH_3S(^2A',C_s)	-0.9984
145	CH_3CH_2(^2A',C_s)	-1.0191
146	$(CH_3)_2CH$(^2A',C_s)	-1.0177
147	$(CH_3)_3C$(t-butyl radical C_{3v})	-1.0168
148	NO_2	-1.0118
149	CH_2=C=$CHCH_3$ (1,2-butadiene)	-0.8075
150	CH_2=CH-$C(CH_3)$=CH_2 (isoprene)	-0.8069
151	C_5H_{10} (cyclopentane)	-0.8060
152	C_5H_{12} (n-pentane)	-0.8065
153	$C(CH_3)_4$ (neopentane)	-0.8063
154	C_6H_8 (1,3-cyclohexadiene)	-0.8062
155	C_6H_8 (1,4-cyclohexadiene)	-0.8061
156	C_6H_{12} (cyclohexane)	-0.8057
157	C_6H_{14} (n-hexane)	-0.8064
158	C_6H_{14} (3-methyl pentane)	-0.8062
159	$C_6H_5CH_3$ (toluene)	-0.8061
160	C_7H_{16} (n-heptane)	-0.8062
161	C_8H_8 (1,3,5,7-cyclooctatetraene)	-0.8062
162	C_8H_{18} (n-octane)	-0.8061
163	$C_{10}H_8$ (naphthalene)	-0.8057
164	$C_{10}H_8$ (azulene)	-0.8058
165	CH_3COOCH_3 (methyl acetate)	-0.8040
166	$(CH_3)_3COH$ (t-butanol)	-0.8049
167	$C_6H_5NH_2$ (aniline)	-0.8054
168	C_6H_5OH (phenol)	-0.8049
169	CH_2=CH-O-CH=CH_2 (divinyl ether)	-0.8054
170	C_4H_8O (tetrahydrofuran)	-0.8047
171	C_5H_8O (cyclopentanone)	-0.8049
172	$C_6H_4O_2$ (1,4-benzoquinone)	-0.8046
173	$C_4H_4N_2$ (pyrimidine)	-0.8052
174	$(CH_3)_2SO_2$ (dimethyl sulfone)	-0.7959
175	C_6H_5Cl (chlorobenzene)	-0.7972
176	NC-CH_2CH_2-CN (succinonitrile)	-0.8065
177	$C_4H_4N_2$ (pyrazine)	-0.8052
178	CH_3COCCH (acetyl acetylene)	-0.8059
179	CH_3-CH=CH-CHO (crotonaledehyde)	-0.8056
180	$(CH_3CO)_2O$ (acetic anhydride)	-0.8037

Table S12 – continued

181	C_4H_6S (25-dihydrothiophene)	-0.7965
182	$CH_3CH(CH_3)CN$ (2-methyl propanenitrile)	-0.8066
183	CH_3-CO-CH_2CH_3 (methyl ethyl ketone)	-0.8053
184	$(CH_3)_2$CH-CHO (isobutyraldehyde)	-0.8054
185	$C_4H_8O_2$ (1,4-dioxane)	-0.8037
186	C_4H_8S (tetrahydrothiophene)	-0.7965
187	$(CH_3)_3$C-Cl (t-butyl chloride)	-0.7959
188	$CH_3CH_2CH_2CH_2Cl$ (n-butyl chloride)	-0.7960
189	C_4H_8NH (pyrrolidine)	-0.8053
190	$CH_3CH_2CH(NO_2)CH_3$ (2-nitrobutane)	-0.8040
191	$CH_3CH_2OCH_2CH_3$ (diethyl ether)	-0.8052
192	CH_3-$CH(OCH_3)_2$ (1,1-dimethoxy ethane)	-0.8041
193	$(CH_3)_3$C-SH (t-butanethiole)	-0.7968
194	$(CH_3CH_2S)_2$ (diethyl disulfide)	-0.7939
195	$(CH_3)_3$C-NH_2 (t-butylamine)	-0.8056
196	$Si(CH_3)_4$ (tetramethyl silane)	-0.7994
197	C_5H_6S (2-methyl thiopehene)	-0.7974
198	C5H7N (N-methyl pyrrole)	-0.8053
199	$C_5H_{10}O$ (tetrahydropyran)	-0.8046
200	$C_2H_5COC_2H_5$ (diethyl ketone)	-0.8053
201	$CH_3COOCH(CH_3)_2$ (isopropyl acetate)	-0.8043
202	$C_5H_{10}S$ (tetrahydrothiopyran)	-0.7974
203	$C_5H_{10}NH$ (piperidine)	-0.8051
204	$(CH_3)_3COCH_3$ (t-butyl methyl ether)	-0.8050
205	$C_6H_4F_2$ (1,3-difluuorobenzene)	-0.8032
206	$C_6H_4F_2$ (1,4-difluuorobenzene)	-0.8032
207	C_6H_5F (fluorobenzene)	-0.8044
208	$(CH_3)_2CHOCH(CH_3)_2$ (diisopropyl ether)	-0.8051
209	PF_5	-0.7955
210	SF_6	-0.7951
211	P_4	-0.7890
212	SO_3	-0.7945
213	SCl_2	-0.7875
214	$POCl_3$	-0.7884
215	PCl_5	-0.7872
216	SO_2Cl_2	-0.7895
217	PCl_3	-0.7875
218	S_2Cl_2	-0.7876
219	$SiCl_2$ ($^1A_1$)	-0.7882
220	CF_3Cl	-0.7942
221	C_2F_6	-0.7997
222	CF_3	-1.0085
223	C_6H_5 (phenyl radical)	-1.0162

IP-EA 13/3

1	C	-1.0267
2	S	-0.9942
3	SH	-0.9940
4	Cl	-0.9924
5	Cl_2	-0.9922
6	OH	-1.0126
7	O	-1.0156
8	O_2	-1.0120
9	P	-0.9959
10	PH	-0.9960

Table S12 – continued

11	PH_2	-0.9959
12	S_2	-0.9933
13	Si	-0.9974

PA8

1	NH_3	-0.8065
2	H_2O	-0.8037
3	HCCH	-0.8099
4	SiH_4	-0.7929
5	PH_3	-0.7909
6	H_2S	-0.7893
7	HCl	-0.7879
8	H_2	-0.8436

HB6/04, CT7/04, DI6/04, WI7/05 and PPS5/05

1	$(NH_3)_2$	-0.8064
2	$(HF)_2$	-0.8011
3	$(H_2O)_2$	-0.8036
4	NH_3-H_2O	-0.8036
5	$(HCONH_2)_2$	-0.8042
6	$(HCOOH)_2$	-0.8033
7	C_2H_4-F2	-0.8010
8	NH_3-F2	-0.8010
9	C_2H_2-ClF	-0.7909
10	HCN-ClF	-0.7909
11	NH_3-Cl2	-0.7874
12	H_2O-ClF	-0.7909
13	NH_3-ClF	-0.7909
14	$(H_2S)_2$	-0.7893
15	$(HCl)_2$	-0.7879
16	HCl-H_2S	-0.7879
17	CH_3Cl-HCl	-0.7879
18	HCN-CH_3SH	-0.7924
19	CH_3SH-HCl	-0.7879
20	HeNe	-0.7989
21	HeAr	-0.7869
22	Ne_2	-0.7989
23	NeAr	-0.7869
24	CH_4-Ne	-0.7989
25	C_6H_6-Ne	-0.8064
26	$(CH_4)_2$	-0.8100
27	$(C_2H_2)_2$	-0.8098
28	$(C_2H_4)_2$	-0.8089
29	Sandwich C_6H_6	-0.8064
30	T-Shaped C_6H_6	-0.8064
31	Parallel C_6H_6	-0.8064

HTBH38/04 (Only the transition state)

1	$H + HCl \rightarrow H_2 + Cl$	-0.9933
2	$OH + H_2 \rightarrow H + H_2O$	-1.0147
3	$CH_3 + H_2 \rightarrow H + CH_4$	-1.0221
4	$OH + CH_4 \rightarrow CH_3 + H_2O$	-1.0153

Table S12 – continued

5	$H + H_2 \rightarrow H_2 + H$	-1.0509
6	$OH + NH_3 \rightarrow H_2O + NH_2$	-1.0134
7	$HCl + CH_3 \rightarrow Cl + CH_4$	-0.9973
8	$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	-1.0153
9	$F + H_2 \rightarrow HF + H$	-1.0122
10	$O + CH_4 \rightarrow OH + CH_3$	-1.0169
11	$H + PH_3 \rightarrow PH_2 + H_2$	-0.9968
12	$H + HO \rightarrow H_2 + O$	-1.0167
13	$H + H_2S \rightarrow H_2 + HS$	-0.9947
14	$O + HCl \rightarrow OH + Cl$	-0.9973
15	$NH_2 + CH_3 \rightarrow CH_4 + NH$	-1.0189
16	$NH_2 + C_2H_5 \rightarrow C_2H_6 + NH$	-1.0177
17	$C_2H_6 + NH_2 \rightarrow NH_3 + C_2H_5$	-1.0166
18	$NH_2 + CH_4 \rightarrow CH_3 + NH_3$	-1.0173
19	$C_5H_8 \rightarrow C_5H_8$	-0.8064

NHTBH38/04 (Only the transition state)

1	$H + N_2O \rightarrow OH + N_2$	-1.0130
2	$H + FH \rightarrow HF + H$	-1.0091
3	$H + ClH \rightarrow + HCl\ H$	-0.9928
4	$H + FCH_3 \rightarrow HF + CH_3$	-1.0126
5	$H + F_2 \rightarrow HF + F$	-1.0093
6	$CH_3 + FCl \rightarrow CH_3F + Cl$	-0.9997
7	$F^- + CH_3F \rightarrow FCH_3 + F^-$	-0.8018
8	$F^- \cdots CH_3F \rightarrow FCH_3 \cdots F^-$	-0.8018
9	$Cl^- + CH_3Cl \rightarrow ClCH_3 + Cl^-$	-0.7894
10	$Cl^- \cdots CH_3Cl \rightarrow ClCH_3 \cdots Cl^-$	-0.7894
11	$F^- + CH_3Cl \rightarrow FCH_3 + Cl^-$	-0.7931
12	$F^- \cdots CH_3Cl \rightarrow FCH_3 \cdots Cl^-$	-0.7931
13	$OH^- + CH_3F \rightarrow HOCH_3 + F^-$	-0.8027
14	$OH^- \cdots CH_3F \rightarrow HOCH_3 \cdots F^-$	-0.8027
15	$H + N_2 \rightarrow HN_2$	-1.0163
16	$H + CO \rightarrow HCO$	-1.0161
17	$H + C2H_4 \rightarrow CH_3CH_2$	-1.0194
18	$CH_3 + C2H_4 \rightarrow CH_3CH_2CH_2$	-1.0190
19	$HCN \rightarrow HNC$	-0.8081

T-96R

1	H_2	-0.8434
2	Li_2	-0.8363
3	LiH	-0.8367
4	LiF	-0.8049
5	LiCl	-0.7901
6	LiO	-1.0206
7	Be2	-0.8301
8	BeH	-1.0464
9	BeF	-1.0148
10	BeO	-0.8085
11	BeS	-0.7919
12	B_2	-1.0339
13	BH	-0.8248
14	BF	-0.8053
15	BF_3	-0.8009
16	BCl	-0.7912

Table S12 – continued

17	BCl_3	-0.7882
18	BN	-1.0233
19	BO	-1.0175
20	BS	-0.9982
21	C_2	-0.8148
22	CH	-1.0305
23	CH_4	-0.8101
24	CF	-1.0139
25	CF_4	-0.7998
26	CCl	-0.9971
27	CCl_4	-0.7878
28	CN	-1.0196
29	CO	-0.8064
30	CO^+	-1.0177
31	CO_2	-0.8036
32	CP	-1.0001
33	CS	-0.7924
34	CS_2	-0.7901
35	N_2	-0.8068
36	N_2^+	-1.0190
37	NH	-1.0215
38	NH^+	-1.0274
39	NF	-1.0124
40	NCl	-0.9969
41	NO	-1.0143
42	NO^+	-0.8061
43	NS	-0.9983
44	O_2	-1.0123
45	O_2^+	-1.0138
46	OH	-1.0155
47	OH^+	-1.0186
48	OF	-1.0110
49	F_2	-0.8009
50	F_2^+	-1.0104
51	HF	-0.8010
52	HF^+	-1.0129
53	Na_2	-0.7965
54	NaH	-0.7976
55	NaF	-0.7981
56	NaCl	-0.7905
57	NaO	-1.0076
58	MgH	-1.0026
59	MgF	-1.0039
60	MgCl	-0.9954
61	MgO	-0.7977
62	Al_2	-0.9990
63	AlH	-0.7941
64	AlF	-0.7954
65	AlCl	-0.7895
66	AlO	-1.0030
67	AlS	-0.9956
68	Si_2	-0.9971
69	SiH	-0.9984
70	SiH_4	-0.7929
71	SiF	-1.0007
72	SiF_4	-0.7962

Table S12 – continued

73	SiCl	-0.9942
74	SiCl	-0.7875
75	SiN	-1.0019
76	SiO	-0.7946
77	SiS	-0.7896
78	P_2	-0.7897
79	P_4	-0.7890
80	PH	-0.9963
81	PF	-0.9992
82	PCl	-0.9934
83	PN	-0.7936
84	PO	-0.9995
85	S_2	-0.9934
86	SH	-0.9945
87	SF	-0.9978
88	SF_6	-0.7952
89	SO	-0.9979
90	SO_3	-0.7945
91	Cl_2	-0.7874
92	Cl_2^+	-0.9923
93	HCl	-0.7879
94	HCl^+	-0.9934
95	ClF	-0.7908
96	ClO	-0.9967

T-82F

1	H_2	-0.8434
2	Li_2	-0.8363
3	LiH	-0.8367
4	LiF	-0.8049
5	LiCl	-0.7901
6	LiO	-1.0205
7	LiNa	-0.8008
8	Be_2	-0.8301
9	BeH	-1.0463
10	BeH^+	-0.8345
11	BeF	-1.0148
12	BeCl	-0.9963
13	BeO	-0.8085
14	BeS	-0.7919
15	B_2	-1.0339
16	BH	-0.8248
17	BF	-0.8053
18	BCl	-0.7912
19	BN	-1.0233
20	BO	-1.0175
21	BS	-0.9982
22	C_2	-0.8127
23	CH	-1.0304
24	CF	-1.0138
25	CN	-1.0196
26	CO	-0.8064
27	CO^+	-1.0176
28	CP	-1.0001
29	CS	-0.7924

Table S12 – continued

30	N_2	-0.8068
31	N_2^+	-1.0190
32	NH	-1.0215
33	NF	-1.0123
34	NCl	-0.9969
35	NO	-1.0143
36	NO^+	-0.8061
37	NS	-0.9983
38	O_2	-1.0123
39	O_2^+	-1.0138
40	OH	-1.0155
41	OH^+	-1.0186
42	F_2	-0.8009
43	F_2^+	-1.0104
44	HF	-0.8010
45	HF^+	-1.0129
46	Na2	-0.7965
47	NaH	-0.7976
48	NaF	-0.7981
49	NaO	-1.0076
50	MgH	-1.0026
51	MgH^+	-0.7960
52	MgO	-0.7977
53	MgS	-0.7908
54	Al_2	-0.9990
55	AlH	-0.7941
56	AlF	-0.7954
57	AlCl	-0.7895
58	AlO	-1.0030
59	AlS	-0.9956
60	Si_2	-0.9971
61	SiH	-0.9984
62	SiH^+	-0.7929
63	SiF	-1.0007
64	SiCl	-0.9941
65	SiN	-1.0018
66	SiO	-0.7946
67	SiS	-0.7896
68	P_2	-0.7897
69	P_2^+	-0.9954
70	PH	-0.9963
71	PF	-0.9991
72	PCl	-0.9934
73	PN	-0.7936
74	PO	-0.9995
75	S_2	-0.9934
76	SO	-0.9979
77	Cl_2	-0.7874
78	Cl_2^+	-0.9922
79	HCl	-0.7879
80	HCl+	-0.9934
81	ClF	-0.7908
82	ClO	-0.9967

Lieb-Oxford bound and the gedanken density of Perdew, Ruzsinszky, Sun, and Burke (J. Chem. Phys. 140, 18A533 (2014))

The gedanken density of Perdew and collaborators is defined as

$$\rho(\mathbf{r}) = \begin{cases} \frac{A}{r^3} & \text{for } R_0 < r < R_1 \\ 0 & \text{otherwise} \end{cases} \tag{S2}$$

and it integrates to two electrons, so that

$$A = \frac{1}{2\,\pi\,ln(y)} \tag{S3}$$

where

$$y = \frac{R_1}{R_0} \tag{S4}$$

This definition implies that the reduced density gradient is equal to

$$s = \frac{3}{2}\left(\frac{2}{3\,\pi} ln(y)\right)^{\frac{1}{3}} \tag{S5}$$

in the interval where the density is different from zero. This expression for the reduced density gradient implies that it is constant in this interval, and therefore

$$E_x^{GGA}[\rho] = -4\,\pi\,A^{\frac{4}{3}}\,\frac{1}{R_0}\left(1-\frac{1}{y}\right)\,\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\,F_x(s) \tag{S6}$$

where s is given by Eq. (S5). Since the Lieb-Oxford bound establishes that

$$E_x^{GGA}[\rho] \geq -1.679 \int \rho(\mathbf{r})^{\frac{4}{3}}\,d\mathbf{r} \tag{S7}$$

then, substituting Eq. (S6) in Eq. (S7), with the integral evaluated for the density given by Eq. (S2), one finds that the Lieb-Oxford bound adopts in this case the form

$$\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\,F_x(s) \leq 1.679 \tag{S8}$$

From Eq. (S8) one can see that if the enhancement function is greater than $1.679/[\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}]$ for a certain value of s determined from Eq. (S5), the Lieb-Oxford bound will be violated. Thus, in the case of enhancement functions that diverge as functions of s, one has the certainty that there will be values of y that do not comply with Eq. (S8).
In particular, in Fig. S1, we present the behavior for the enhancement function given by Eq. (14) of the manuscript. This plot shows that for values of $ln(y) \geq 85.207$, the Lieb-Oxford bound is violated.

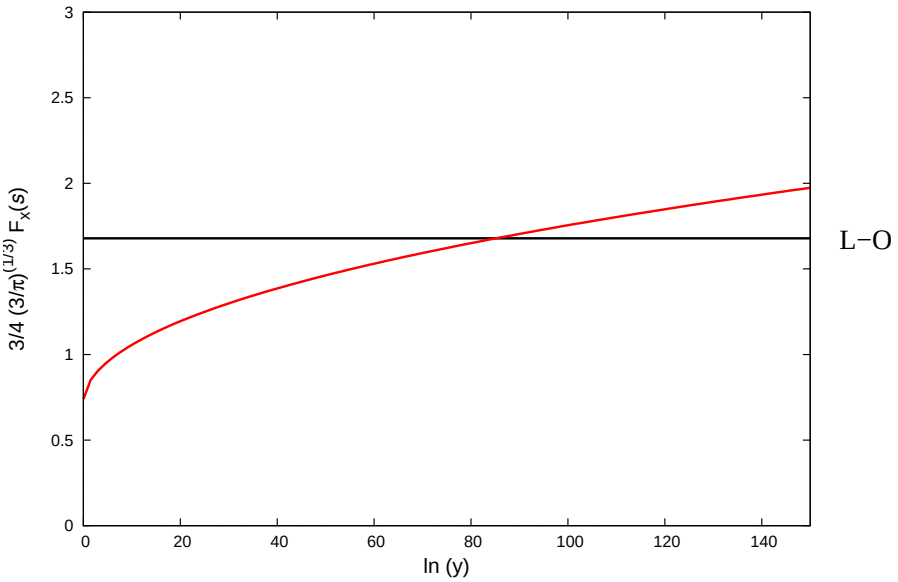

Figure S1: Plot of the enhancement function with s given by Eq. (S5) as a function of $ln(y)$. The Lieb-Oxford (L-O) bound of 1.679 is indicated with the straight line. Densities that lie below this line comply with the bound, while densities that lie above violate the bound.