Supplementary Material to: Assessment of Density Functional Methods for Exciton Binding Energies and Related Optoelectronic Properties

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Table S1. Vertical ionization potentials (1) [in eV] of the 121 molecules studied. Most experimental reference values are collected from the NIST database,[1] while other publications[2-13] are adopted for the molecules marked.

Molecule	Expt.	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	5.99	5.93	6.46	6.08	5.89	6.02	5.89	5.95	6.00	5.79	5.84
AlCl3 (Aluminum trichloride)	12.01	12.25	11.55	10.88	11.13	11.32	12.20	12.02	11.76	11.89	12.41
Ar (Argon atom)	15.76	15.68	16.51	15.71	15.79	15.79	15.73	15.75	15.78	15.78	15.73
B (Boron atom)	8.30	8.19	9.09	8.67	8.61	8.74	8.40	8.51	8.56	8.31	8.10
BCl3 (Borane, trichloro-)	11.64	11.98	11.47	10.80	11.07	11.22	11.95	11.79	11.56	11.72	12.20
Be (Beryllium atom)[11]	9.32	9.29	9.46	9.00	8.93	9.11	8.92	8.87	8.84	9.06	9.08
BF3 (Borane, trifluoro-)	15.96	16.34	15.28	14.44	14.51	15.22	15.57	15.52	15.38	16.04	17.28
C (Carbon atom)	11.26	11.18	12.14	11.54	11.39	11.54	11.29	11.39	11.44	11.31	11.18
C2F4 (Tetrafluoroethylene)	10.69	10.76	10.92	10.08	10.00	10.48	10.36	10.41	10.41	10.73	11.29
C2H2 (Acetylene)	11.49	11.33	12.25	11.41	11.17	11.35	11.20	11.24	11.27	11.36	11.62
C2H2O2 (Ethanedial)	10.60	10.86	10.68	9.99	10.02	10.47	10.74	10.70	10.58	10.82	11.48
C2H4 (Ethylene)	10.68	10.50	11.45	10.62	10.38	10.53	10.37	10.41	10.43	10.46	10.55
C2H4O (Ethylene oxide)	10.57	10.68	11.20	10.47	10.40	10.60	10.63	10.61	10.58	10.77	11.04
C2H4S (Thiirane)	9.05	9.02	9.64	8.92	8.94	9.00	8.98	9.00	9.01	9.10	9.27
C2H5N (Aziridine)	9.85	9.79	10.33	9.63	9.61	9.73	9.75	9.73	9.71	9.90	10.13
C2H6 (Ethane)	11.99	12.83	12.42	11.91	12.11	12.28	12.53	12.46	12.36	12.54	12.90
C2HF3 (Trifluoroethylene)[5]	10.62	10.50	10.82	10.00	9.93	10.28	10.16	10.21	10.21	10.46	10.88
C2N2 (Cyanogen)	13.51	13.59	13.98	13.14	13.03	13.25	13.39	13.37	13.32	13.57	14.01
C3H4 (Cyclopropene)	9.86	9.90	10.41	9.72	9.63	9.76	9.72	9.73	9.72	9.89	10.19
C3H6 (Cyclopropane)	10.54	10.90	11.50	10.75	10.76	10.82	10.83	10.82	10.80	10.96	11.06
C3H8 (Propane)	11.51	12.23	11.59	11.09	11.32	11.55	11.91	11.82	11.67	11.87	12.36
C3O2 (Carbon suboxide)[10]	10.80	10.69	11.60	10.76	10.60	10.86	10.69	10.74	10.79	11.00	11.42
C4H2 (Diacetylene)	10.30	10.23	10.70	9.92	9.86	9.98	10.02	10.02	10.00	10.21	10.57
C4H4O (Furan)	8.90	8.93	9.70	8.90	8.76	8.89	8.84	8.85	8.85	9.02	9.30
C4H6 (Cyclobutene)	9.43	9.56	10.14	9.41	9.27	9.43	9.36	9.37	9.38	9.51	9.73
C4N2 (2-Butynedinitrile)[4]	11.84	12.11	12.31	11.51	11.45	11.67	11.89	11.86	11.79	12.05	12.56
CCl4 (Carbon tetrachloride)	11.69	11.91	11.19	10.54	10.83	11.03	11.87	11.68	11.41	11.62	12.20
CF2Cl2 (Difluorodichloromethane)	12.24	12.43	12.20	11.49	11.72	11.89	12.37	12.27	12.12	12.29	12.65
CF2O (Carbonic difluoride)	13.60	13.58	14.05	13.16	13.07	13.47	13.45	13.44	13.43	13.70	14.10
CF3Br (Bromotrifluoromethane)[8]	12.08	12.04	12.45	11.64	11.50	11.93	11.86	11.89	11.89	11.95	12.45
CF3Cl (Methane, chlorotrifluoro-)	13.08	13.10	13.32	12.55	12.69	12.93	13.00	13.01	12.99	13.15	13.38
CF4 (Carbon tetrafluoride)	16.20	16.77	15.36	14.54	14.72	15.47	15.82	15.79	15.65	16.44	17.84

CFCl3 (Trichloromonofluoromethane)	11.76	12.02	11.50	10.83	11.10	11.27	11.98	11.82	11.59	11.78	12.26
CH2CCH2 (Allene)	10.20	10.15	10.84	10.08	9.90	10.10	10.03	10.05	10.06	10.16	10.41
CH2CCl2 (Ethene, 1,1-dichloro-)	10.00	10.00	10.29	9.56	9.55	9.72	9.88	9.84	9.78	9.91	10.22
CH2CF2 (Ethene, 1,1-difluoro-)[5]	10.70	10.67	11.20	10.37	10.24	10.55	10.42	10.46	10.47	10.67	11.02
CH2CHCHO (Acrolein)[13]	10.10	10.11	10.55	9.80	9.72	9.96	10.01	9.99	9.95	10.15	10.48
CH2CHCl (Ethene, chloro-)	10.20	10.11	10.57	9.83	9.81	9.92	9.99	9.97	9.94	10.05	10.27
CH2CHF (Ethene, fluoro-)	10.63	10.52	11.18	10.36	10.24	10.44	10.31	10.35	10.36	10.49	10.71
CH2Cl2 (Methylene chloride)	11.40	11.66	11.31	10.69	10.89	11.23	11.65	11.57	11.44	11.55	11.82
CH2CO (Ketene)	9.64	9.68	10.53	9.72	9.55	9.80	9.69	9.72	9.74	9.87	10.20
CH2F2 (Methane, difluoro-)	13.27	13.69	13.07	12.42	12.53	13.01	13.13	13.12	13.05	13.43	14.19
CH3 (Methyl radical)	9.84	9.71	10.55	10.02	9.85	9.92	9.72	9.76	9.77	9.76	9.69
CH3CCCH3 (2-Butyne)	9.79	9.64	9.99	9.30	9.23	9.41	9.42	9.43	9.41	9.60	9.93
CH3CCH (Propyne)	10.37	10.39	10.95	10.21	10.08	10.26	10.21	10.23	10.23	10.38	10.69
CH3CH2Cl (Ethyl chloride)	11.06	11.12	11.70	10.66	10.81	10.94	11.07	11.06	11.02	11.13	11.28
CH3CH2OH (Ethanol)	10.64	10.75	10.82	10.19	10.21	10.52	10.63	10.60	10.53	10.75	11.13
CH3Cl (Methyl chloride)	11.29	11.38	11.75	11.09	11.21	11.27	11.34	11.33	11.32	11.40	11.54
CH3COCl (Acetyl Chloride)	11.03	11.23	11.47	10.74	10.77	10.95	11.07	11.04	10.99	11.14	12.08
CH3F (Methyl fluoride)	13.04	13.46	13.36	12.71	12.78	13.08	13.15	13.13	13.08	13.32	13.80
CH3NHCH3 (Dimethylamine)	8.95	8.99	9.44	8.77	8.75	8.92	8.96	8.94	8.90	9.08	9.31
CH3NO2 (Methane, nitro-)	11.29	11.41	11.76	11.00	11.01	11.45	11.69	11.64	11.53	11.90	12.65
CH3OCH3 (Dimethyl ether)	10.10	10.11	10.39	9.73	9.72	9.94	10.01	9.98	9.94	10.14	10.44
CH3OH (Methyl alcohol)	10.96	11.02	11.38	10.68	10.63	10.89	10.93	10.91	10.87	11.06	11.41
CH3SH (Methanethiol)	9.44	9.39	9.95	9.26	9.28	9.36	9.35	9.38	9.38	9.44	9.54
CH3SiH3 (Methyl silane)	11.60	11.73	11.80	11.25	11.45	11.57	12.17	12.11	12.00	11.70	12.28
CH4 (Methane)	13.60	14.38	14.58	13.96	14.05	14.18	14.18	14.18	14.16	14.29	14.58
CHCl3 (Chloroform)	11.50	11.63	11.18	10.52	10.78	10.92	11.61	11.45	11.23	11.41	11.83
CHF3 (Methane, trifluoro-)	15.50	14.97	14.25	13.52	13.60	14.19	14.36	14.34	15.18	14.69	15.54
CHONH2 (Formamide)[3]	10.40	10.31	11.01	10.22	10.04	10.31	10.27	10.25	10.24	10.41	10.72
Cl (Chlorine atom)	12.97	12.84	13.40	12.97	12.88	13.07	12.96	13.01	13.04	13.00	13.09
Cl2 (Chlorine diatomic)	11.49	11.64	11.87	11.18	11.35	11.42	11.66	11.60	11.54	11.64	11.82
ClF (Chlorine monofluoride)	12.77	12.81	13.16	12.41	12.51	12.71	12.72	12.74	12.74	12.93	13.20
ClF3 (Chlorine trifluoride)	13.05	13.24	12.74	11.98	12.11	12.66	12.88	12.87	12.77	13.23	14.07
ClO (Monochlorine monoxide)	11.01	11.03	11.19	10.75	10.72	11.04	11.06	11.06	11.04	11.13	11.46
CO (Carbon monoxide)	14.01	14.01	14.60	13.86	13.66	14.19	14.18	14.14	14.11	14.13	14.57
CO2 (Carbon dioxide)	13.78	13.77	14.55	13.67	13.52	13.81	13.84	13.82	13.80	14.03	14.44
CS (Carbon monosulfide)[9]	11.34	11.35	11.99	11.29	11.10	11.49	11.53	11.49	11.48	11.43	11.77
CS2 (Carbon disulfide)	10.09	9.97	10.74	10.03	10.05	10.06	10.00	10.03	10.08	10.15	10.31

F (Fluorine atom)	17.42	17.28	18.52	17.66	17.21	17.73	17.46	17.45	17.47	17.50	17.54
F2 (Fluorine diatomic)	15.70	16.08	16.18	15.35	15.42	15.92	15.81	15.87	15.88	16.28	16.83
F2O (Difluorine monoxide)	13.26	13.55	13.48	12.69	12.76	13.37	13.32	13.36	13.34	13.75	14.45
FCN (Cyanogen fluoride)[3]	13.65	13.52	14.19	13.31	13.16	13.43	13.30	13.34	13.36	13.59	13.94
H (Hydrogen atom)	13.60	13.60	13.51	13.60	13.71	13.67	13.65	13.65	13.68	13.57	13.53
H2CO (Formaldehyde)	10.89	10.88	11.45	10.75	10.69	10.89	10.83	10.84	10.83	10.99	11.28
H2CS (Thioformaldehyde)	9.38	9.32	9.95	9.25	9.22	9.32	9.25	9.29	9.32	9.40	9.64
H2O (Water)[6]	12.62	12.63	13.70	12.80	12.44	12.81	12.71	12.69	12.68	12.78	13.03
H2O2 (Hydrogen peroxide)	11.70	11.79	12.04	11.29	11.29	11.67	11.68	11.68	11.64	11.92	12.37
H2S (Hydrogen sulfide)	10.50	10.38	11.15	10.41	10.39	10.46	10.40	10.43	10.46	10.47	10.50
HCCCN (Cyanoacetylene)[2]	11.75	11.70	12.17	11.37	11.27	11.44	11.50	11.50	11.47	11.69	12.08
HCCF (Fluoroacetylene)[5]	11.50	11.34	12.00	11.16	11.03	11.26	11.13	11.17	11.19	11.39	11.73
HCl (Hydrogen sulfide)[12]	12.77	12.69	13.50	12.73	12.73	12.78	12.72	12.75	12.78	12.79	12.85
HCN (Hydrogen cyanide)	13.61	13.62	14.64	13.75	13.46	13.68	13.51	13.55	13.58	13.66	13.90
HCO (Formyl radical)	9.31	9.68	10.27	9.77	9.74	10.06	9.90	9.95	9.96	9.96	10.23
HCOOH (Formic acid)	11.50	11.26	11.93	11.10	10.92	11.24	11.21	11.19	11.17	11.37	11.74
He (Helium atom)	24.59	24.56	24.78	24.47	24.69	24.94	24.66	24.66	24.72	24.72	24.76
HF (Hydrogen fluoride)	16.12	16.12	17.30	16.32	15.88	16.33	16.21	16.16	16.16	16.21	16.41
Li (Lithium atom)	5.39	5.34	5.88	5.58	5.10	5.63	5.33	5.30	5.37	5.41	5.83
Mg (Magnesium atom)	7.65	7.53	8.15	7.61	7.53	7.73	7.64	7.59	7.47	7.77	7.74
N (Nitrogen atom)	14.53	14.47	15.46	14.73	14.68	14.66	14.52	14.57	14.61	14.53	14.33
N2 (Nitrogen diatomic)	15.58	15.71	16.14	15.39	15.32	15.83	15.89	15.90	15.87	16.07	16.84
N2H4 (Hydrazine)	8.98	9.84	10.03	9.39	9.45	9.64	9.71	9.69	9.64	9.85	10.18
N2O (Nitrous oxide)	12.89	12.77	13.79	12.90	12.71	12.93	12.77	12.79	12.83	12.98	13.15
Na (Sodium atom)	5.14	4.68	5.78	5.36	4.49	5.43	4.88	4.88	4.97	5.16	5.62
NaCl (Sodium Chloride)	9.80	9.12	10.10	9.32	9.20	9.33	9.19	9.22	9.25	9.29	9.39
Ne (Neon atom)	21.57	21.46	22.74	21.66	21.18	21.71	21.53	21.47	21.49	21.50	21.67
NF3 (Nitrogen trifluoride)	13.60	13.73	13.70	12.92	12.94	13.43	13.43	13.44	13.40	13.74	14.31
NH (Imidogen) (3^−)	13.49	13.44	14.44	13.79	13.60	13.72	13.55	13.58	13.61	13.58	13.51
NH2 (Amino radical)	12.00	11.96	12.86	12.18	11.79	12.26	12.12	12.07	12.06	11.98	12.10
NH3 (Ammonia)	10.82	10.85	11.77	10.96	10.67	11.00	10.92	10.90	10.90	10.96	11.19
NO (Nitric oxide)	9.26	9.80	10.36	9.90	9.77	10.27	10.01	10.09	10.12	10.14	10.57
NO2 (Nitrogen dioxide)	11.23	11.57	11.81	11.17	11.06	11.71	11.65	11.68	11.65	11.88	12.70
O (Oxygen atom)	13.62	13.46	14.57	14.06	13.65	14.14	13.81	13.80	13.79	13.68	13.77
O2 (Oxygen diatomic) (3^g)	12.30	12.61	13.27	12.55	12.63	13.02	12.83	12.90	12.93	13.10	13.48
O3 (Ozone)	12.73	13.29	13.41	12.61	12.52	13.14	13.22	13.22	13.15	13.58	14.56
OCS (Carbonyl sulfide)	11.19	11.20	12.02	11.24	11.22	11.31	11.22	11.26	11.31	11.38	11.57
OH (Hydroxyl radical)	13.02	12.97	14.07	13.30	12.90	13.34	13.14	13.13	13.13	13.13	13.19

P (Phosphorus atom)	10.49	10.45	11.02	10.49	10.58	10.39	10.39	10.40	10.42	10.32	10.16
P2 (Phosphorus diatomic)	10.62	10.44	11.22	10.51	10.43	10.44	10.29	10.85	10.84	10.44	10.54
PF3 (Phosphorus trifluoride)	12.20	11.74	12.06	11.27	11.25	11.62	11.55	11.59	11.57	11.67	12.00
PH3 (Phosphine)	10.59	10.53	11.15	10.48	10.54	10.59	10.49	10.53	10.56	10.50	10.37
S (Sulfur atom)	10.36	10.21	11.08	10.43	10.22	10.56	10.39	10.46	10.50	10.43	10.51
S2 (Sulfur diatomic) (3^g)	9.55	9.52	10.00	9.46	9.56	9.62	9.83	9.76	9.70	9.66	9.77
Si (Silicon atom)	8.15	8.09	8.41	8.20	8.06	8.11	8.04	8.08	8.12	7.98	7.99
Si2H6 (Disilane)	10.53	10.56	10.89	10.27	10.34	10.44	10.47	10.48	10.46	10.48	10.48
SiF2 (Silicon difluoride)	11.08	11.10	11.56	10.81	10.80	11.07	11.05	11.05	11.03	10.99	11.07
SiF4 (Silicon tetrafluoride)	16.40	16.91	15.27	14.45	14.57	15.36	15.95	15.85	15.63	16.40	17.89
SiH3 (Silyl)	8.74	8.84	9.40	8.95	8.87	8.96	8.79	8.85	8.88	8.91	8.92
SiH4 (Silane)	12.30	12.86	12.67	12.14	12.37	12.47	12.74	12.67	12.58	12.59	12.82
SiO (Silicon monoxide)[7]	11.61	11.51	12.02	11.29	11.23	11.47	11.51	11.53	11.51	11.55	11.85
SO2 (Sulfur dioxide)	12.50	12.58	12.86	12.08	12.01	12.42	12.51	12.51	12.46	12.66	13.26
MAE[a]			0.56	0.35	0.36	0.23	0.20	0.19	0.19	0.18	0.46
MSE[a]			0.45	-0.25	-0.30	-0.03	-0.01	-0.01	-0.03	0.09	0.41
RMS[a]			0.63	0.51	0.48	0.33	0.28	0.27	0.26	0.27	0.60
MAE[b]			0.58	0.42	0.39	0.26	0.16	0.17	0.20	0.13	0.37
MSE[b]			0.39	-0.31	-0.36	-0.09	-0.07	-0.07	-0.09	0.03	0.35
RMS[c]			0.66	0.61	0.56	0.37	0.23	0.24	0.28	0.18	0.46

[a] The reference values are experimental data.

[b] The reference values are calculated by CCSD.

Table S2. Vertical ionization potentials (2) [in eV] of the 121 molecules studied. Most experimental reference values are collected from the NIST database[1], while other publications[2-13] are adopted for the molecules marked.

Molecule	Expt.	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	5.99	5.93	3.43	3.09	3.05	3.63	5.89	5.78	5.48	4.31	5.50
AlCl3 (Aluminum trichloride)	12.01	12.25	8.63	8.01	8.25	9.13	12.17	11.86	11.30	10.74	12.86
Ar (Argon atom)	15.76	15.68	10.89	10.29	10.58	11.67	14.89	14.56	13.93	13.54	16.05
B (Boron atom)	8.30	8.19	4.54	4.17	4.35	5.16	7.90	7.72	7.23	6.16	7.57
BCl3 (Borane, trichloro-)	11.64	11.98	8.33	7.72	7.96	8.85	11.90	11.59	11.03	10.49	12.73
Be (Beryllium atom)[11]	9.32	9.29	6.04	5.61	5.67	6.32	8.78	8.63	8.29	7.25	8.66
BF3 (Borane, trifluoro-)	15.96	16.34	10.80	10.05	10.32	11.94	14.97	14.78	14.20	14.52	18.16
C (Carbon atom)	11.26	11.18	6.56	6.10	6.21	7.33	10.36	10.12	9.55	8.83	11.11
C2F4 (Tetrafluoroethylene)	10.69	10.76	7.03	6.29	6.32	7.59	10.38	10.16	9.64	9.23	11.78
C2H2 (Acetylene)	11.49	11.33	7.84	7.20	7.31	8.19	11.19	10.91	10.35	9.73	11.81
C2H2O2 (Ethanedial)	10.60	10.86	7.01	6.38	6.53	7.77	10.60	10.39	9.85	9.53	12.15
C2H4 (Ethylene)	10.68	10.50	7.40	6.74	6.78	7.63	10.54	10.27	9.74	9.11	11.04
C2H4O (Ethylene oxide)	10.57	10.68	6.88	6.28	6.47	7.71	10.69	10.45	9.88	9.73	12.62
C2H4S (Thiirane)	9.05	9.02	5.93	5.36	5.47	6.36	9.27	8.99	8.46	7.81	9.94
C2H5N (Aziridine)	9.85	9.79	6.36	5.78	5.95	6.97	9.93	9.66	9.11	8.64	11.00
C2H6 (Ethane)	11.99	12.83	8.64	8.18	8.46	9.45	12.42	12.14	11.58	11.03	13.32
C2HF3 (Trifluoroethylene)[5]	10.62	10.50	6.92	6.21	6.26	7.41	10.20	9.97	9.46	8.98	11.34
C2N2 (Cyanogen)	13.51	13.59	10.13	9.40	9.49	10.44	13.33	13.06	12.53	12.00	14.20
C3H4 (Cyclopropene)	9.86	9.90	6.71	6.11	6.20	7.05	9.88	9.62	9.11	8.51	10.51
C3H6 (Cyclopropane)	10.54	10.90	7.71	7.07	7.19	8.15	11.10	10.82	10.27	9.61	11.66
C3H8 (Propane)	11.51	12.23	8.21	7.75	8.01	9.00	11.93	11.65	11.10	10.55	12.74
C3O2 (Carbon suboxide)[10]	10.80	10.69	7.98	7.26	7.31	8.24	10.78	10.60	10.19	9.65	11.75
C4H2 (Diacetylene)	10.30	10.23	7.31	6.64	6.70	7.50	10.23	9.98	9.51	8.90	10.83
C4H4O (Furan)	8.90	8.93	6.35	5.67	5.67	6.49	9.18	8.96	8.49	7.83	9.68
C4H6 (Cyclobutene)	9.43	9.56	6.66	6.04	6.10	6.92	9.73	9.48	8.98	8.37	10.30
C4N2 (2-Butynedinitrile)[4]	11.84	12.11	9.16	8.44	8.50	9.36	12.06	11.82	11.34	10.79	12.84
CCl4 (Carbon tetrachloride)	11.69	11.91	8.29	7.68	7.93	8.84	11.90	11.58	11.01	10.48	12.73
CF2Cl2 (Difluorodichloromethane)	12.24	12.43	8.70	8.07	8.30	9.28	12.34	12.02	11.44	10.94	13.24
CF2O (Carbonic difluoride)	13.60	13.58	9.25	8.51	8.71	10.13	13.16	12.92	12.33	12.32	15.42
CF3Br (Bromotrifluoromethane)[8]	12.08	12.04	8.49	7.83	7.98	8.98	11.90	11.65	11.12	10.57	12.81
CF3Cl (Methane, chlorotrifluoro-)	13.08	13.10	9.20	8.55	8.76	9.84	12.95	12.64	12.04	11.60	14.05
CF4 (Carbon tetrafluoride)	16.20	16.77	11.15	10.40	10.70	12.35	15.38	15.19	14.61	14.97	18.67
CFCl3	11.76	12.02	8.35	7.74	7.98	8.91	11.97	11.65	11.08	10.56	12.84

(Trichloromonofluoromethane)											
CH2CCH2 (Allene)	10.20	10.15	7.19	6.57	6.63	7.51	10.37	10.11	9.59	8.95	10.96
CH2CCl2 (Ethene, 1,1-dichloro-)	10.00	10.00	7.08	6.44	6.53	7.37	10.17	9.92	9.42	8.78	10.75
CH2CF2 (Ethene, 1,1-difluoro-)[5]	10.70	10.67	7.25	6.56	6.63	7.66	10.51	10.27	9.74	9.22	11.44
CH2CHCHO (Acrolein)[13]	10.10	10.11	6.62	6.00	6.19	7.40	10.35	10.12	9.56	9.33	11.72
CH2CHCl (Ethene, chloro-)	10.20	10.11	7.06	6.42	6.51	7.34	10.17	9.91	9.41	8.78	10.73
CH2CHF (Ethene, fluoro-)	10.63	10.52	7.19	6.52	6.59	7.54	10.41	10.16	9.64	9.07	11.16
CH2Cl2 (Methylene chloride)	11.40	11.66	7.95	7.38	7.56	8.55	11.58	11.28	10.71	10.15	12.37
CH2CO (Ketene)	9.64	9.68	6.57	5.91	5.97	6.93	9.71	9.48	8.99	8.39	10.47
CH2F2 (Methane, difluoro-)	13.27	13.69	8.73	8.14	8.38	9.76	12.73	12.50	11.92	11.78	14.77
CH3 (Methyl radical)	9.84	9.71	5.83	5.43	5.54	6.47	9.41	9.15	8.58	7.84	9.48
CH3CCCH3 (2-Butyne)	9.79	9.64	6.53	5.93	6.05	6.90	9.76	9.50	8.98	8.38	10.38
CH3CCH (Propyne)	10.37	10.39	7.11	6.49	6.60	7.48	10.40	10.13	9.59	8.98	11.03
CH3CH2Cl (Ethyl chloride)	11.06	11.12	7.54	6.97	7.16	8.12	11.16	10.85	10.28	9.73	11.92
CH3CH2OH (Ethanol)	10.64	10.75	6.75	6.16	6.35	7.60	10.61	10.35	9.77	9.53	12.24
CH3Cl (Methyl chloride)	11.29	11.38	7.67	7.11	7.31	8.27	11.30	10.99	10.43	9.87	12.10
CH3COCl (Acetyl Chloride)	11.03	11.23	7.77	7.12	7.32	8.39	11.25	11.02	10.50	10.14	12.52
CH3F (Methyl fluoride)	13.04	13.46	8.67	8.09	8.37	9.68	12.68	12.44	11.87	11.71	14.51
CH3NHCH3 (Dimethylamine)	8.95	8.99	5.61	5.07	5.25	6.27	9.19	8.92	8.38	7.94	10.23
CH3NO2 (Methane, nitro-)	11.29	11.41	7.59	6.91	7.08	8.49	11.50	11.27	10.69	10.65	12.90
CH3OCH3 (Dimethyl ether)	10.10	10.11	6.41	5.84	6.04	7.21	10.13	9.89	9.34	9.08	11.68
CH3OH (Methyl alcohol)	10.96	11.02	6.85	6.26	6.47	7.72	10.73	10.48	9.90	9.68	12.43
CH3SH (Methanethiol)	9.44	9.39	6.12	5.56	5.71	6.58	9.51	9.22	8.69	8.00	9.97
CH3SiH3 (Methyl silane)	11.60	11.73	8.48	7.91	8.10	9.00	11.93	11.66	11.12	10.38	12.35
CH4 (Methane)	13.60	14.38	9.96	9.46	9.75	10.78	13.90	13.59	12.98	12.44	14.83
CHCl3 (Chloroform)	11.50	11.63	8.02	7.41	7.65	8.55	11.59	11.28	10.72	10.18	12.41
CHF3 (Methane, trifluoro-)	15.50	14.97	9.98	9.33	9.53	11.00	13.96	13.73	13.15	13.05	16.13
CHONH2 (Formamide)[3]	10.40	10.31	6.64	6.02	6.16	7.42	10.37	10.12	9.56	9.37	11.80
Cl (Chlorine atom)	12.97	12.84	8.49	8.14	8.18	9.35	12.44	12.13	11.55	10.94	13.41
Cl2 (Chlorine diatomic)	11.49	11.64	7.90	7.31	7.46	8.46	11.48	11.18	10.63	10.05	12.35
ClF (Chlorine monofluoride)	12.77	12.81	8.48	7.85	8.03	9.23	12.31	12.02	11.43	11.03	13.65
ClF3 (Chlorine trifluoride)	13.05	13.24	8.67	7.99	8.17	9.62	12.65	12.40	11.82	11.72	14.83
ClO (Monochlorine monoxide)	11.01	11.03	6.69	6.28	6.32	7.72	10.71	10.46	9.89	9.49	12.40
CO (Carbon monoxide)	14.01	14.01	9.60	9.04	9.21	10.53	13.73	13.42	12.79	12.27	15.08
CO2 (Carbon dioxide)	13.78	13.77	9.81	9.09	9.23	10.46	13.38	13.15	12.61	12.34	15.02
CS (Carbon monosulfide)[9]	11.34	11.35	7.92	7.39	7.52	8.68	11.79	11.50	10.92	10.19	12.68
CS2 (Carbon disulfide)	10.09	9.97	7.42	6.82	6.98	7.62	10.21	9.98	9.58	8.81	10.42
F (Fluorine atom)	17.42	17.28	10.89	10.31	10.46	12.29	15.37	15.15	14.53	14.85	18.65

F2 (Fluorine diatomic)	15.70	16.08	10.15	9.46	9.77	11.53	14.56	14.38	13.78	14.20	18.02
F2O (Difluorine monoxide)	13.26	13.55	8.37	7.69	7.89	9.69	12.74	12.53	11.92	12.17	16.05
FCN (Cyanogen fluoride)[3]	13.65	13.52	9.45	8.73	8.85	9.97	12.99	12.71	12.13	11.70	14.13
H (Hydrogen atom)	13.60	13.60	7.80	7.59	7.95	8.78	11.91	11.62	11.06	10.30	12.23
H2CO (Formaldehyde)	10.89	10.88	6.83	6.26	6.48	7.67	10.56	10.34	9.80	9.54	12.29
H2CS (Thioformaldehyde)	9.38	9.32	6.08	5.53	5.63	6.53	9.41	9.14	8.63	7.95	10.10
H2O (Water)[6]	12.62	12.63	7.88	7.25	7.43	8.84	11.99	11.70	11.07	11.00	14.08
H2O2 (Hydrogen peroxide)	11.70	11.79	7.08	6.45	6.62	8.10	11.20	10.94	10.32	10.29	13.54
H2S (Hydrogen sulfide)	10.50	10.38	6.88	6.31	6.45	7.33	10.32	10.02	9.48	8.76	10.72
HCCCN (Cyanoacetylene)[2]	11.75	11.70	8.56	7.87	7.94	8.80	11.60	11.35	10.85	10.27	12.32
HCCF (Fluoroacetylene)[5]	11.50	11.34	7.68	7.01	7.11	8.11	11.06	10.80	10.25	9.71	11.95
HCl (Hydrogen sulfide)[12]	12.77	12.69	8.63	8.05	8.24	9.24	12.36	12.04	11.44	10.89	13.18
HCN (Hydrogen cyanide)	13.61	13.62	9.68	9.02	9.16	10.13	13.24	12.93	12.33	11.80	14.08
HCO (Formyl radical)	9.31	9.68	5.58	5.16	5.23	6.52	9.38	9.16	8.61	8.05	10.63
HCOOH (Formic acid)	11.50	11.26	7.39	6.72	6.85	8.16	11.13	10.89	10.32	10.15	13.08
He (Helium atom)	24.59	24.56	16.02	15.76	16.54	18.00	21.13	20.91	20.28	20.61	24.16
HF (Hydrogen fluoride)	16.12	16.12	10.31	9.65	9.89	11.55	14.68	14.44	13.82	14.12	17.77
Li (Lithium atom)	5.39	5.34	3.58	3.22	3.22	3.65	5.34	5.31	5.20	4.17	5.20
Mg (Magnesium atom)	7.65	7.53	5.20	4.70	4.72	5.30	7.35	7.32	7.08	6.18	7.40
N (Nitrogen atom)	14.53	14.47	8.85	8.30	8.59	9.78	12.93	12.70	12.10	11.76	14.41
N2 (Nitrogen diatomic)	15.58	15.71	10.90	10.27	10.35	11.97	15.13	14.87	14.25	13.95	17.18
N2H4 (Hydrazine)	8.98	9.84	5.84	5.30	5.48	6.62	9.64	9.36	8.77	8.39	10.99
N2O (Nitrous oxide)	12.89	12.77	9.12	8.40	8.47	9.62	12.40	12.19	11.70	11.29	13.78
Na (Sodium atom)	5.14	4.68	3.50	3.04	2.96	3.49	4.83	4.93	4.89	4.19	5.20
NaCl (Sodium Chloride)	9.80	9.12	5.86	5.27	5.26	6.32	9.20	8.91	8.36	7.79	9.99
Ne (Neon atom)	21.57	21.46	14.06	13.35	13.74	15.65	18.64	18.51	17.92	18.69	22.84
NF3 (Nitrogen trifluoride)	13.60	13.73	9.10	8.43	8.57	10.08	13.07	12.83	12.24	12.11	15.28
NH (Imidogen) (3^−)	13.49	13.44	8.41	7.92	8.13	9.36	12.47	12.21	11.61	11.28	13.96
NH2 (Amino radical)	12.00	11.96	7.70	7.22	7.32	8.56	11.64	11.33	10.72	10.29	12.95
NH3 (Ammonia)	10.82	10.85	6.75	6.18	6.37	7.51	10.62	10.31	9.70	9.33	11.90
NO (Nitric oxide)	9.26	9.80	4.95	4.52	4.50	6.18	9.12	8.89	8.31	8.04	11.39
NO2 (Nitrogen dioxide)	11.23	11.57	7.05	6.49	6.46	8.17	11.11	10.89	10.31	10.12	13.55
O (Oxygen atom)	13.62	13.46	7.98	7.60	7.75	9.27	12.35	12.07	11.42	11.22	14.11
O2 (Oxygen diatomic) (3^g)	12.30	12.61	7.40	6.82	7.08	8.72	11.73	11.52	10.93	11.00	14.52
O3 (Ozone)	12.73	13.29	8.71	8.00	8.07	9.69	12.72	12.49	11.89	11.66	13.75
OCS (Carbonyl sulfide)	11.19	11.20	8.14	7.50	7.65	8.47	11.23	10.99	10.53	9.85	11.75
OH (Hydroxyl radical)	13.02	12.97	7.93	7.39	7.44	9.01	12.13	11.85	11.21	11.11	14.41
P (Phosphorus atom)	10.49	10.45	6.74	6.30	6.43	7.12	10.07	9.79	9.26	8.37	10.07

P2 (Phosphorus diatomic)	10.62	10.44	7.72	7.14	7.22	7.85	10.50	10.30	9.90	9.00	10.53
PF3 (Phosphorus trifluoride)	12.20	11.74	7.98	7.34	7.45	8.56	11.41	11.17	10.64	10.04	12.35
PH3 (Phosphine)	10.59	10.53	7.24	6.71	6.87	7.67	10.51	10.26	9.77	8.96	10.74
S (Sulfur atom)	10.36	10.21	6.66	6.16	6.14	7.21	10.09	9.84	9.33	8.53	10.60
S2 (Sulfur diatomic) (3^g)	9.55	9.52	6.29	5.82	5.89	6.81	9.72	9.43	8.90	8.13	10.21
Si (Silicon atom)	8.15	8.09	4.79	4.61	4.57	5.29	7.94	7.74	7.31	6.25	7.82
Si2H6 (Disilane)	10.53	10.56	7.72	7.18	7.33	8.09	10.81	10.58	10.11	9.28	11.11
SiF2 (Silicon difluoride)	11.08	11.10	7.73	7.12	7.21	8.15	10.86	10.67	10.20	9.43	11.32
SiF4 (Silicon tetrafluoride)	16.40	16.91	11.44	10.68	10.95	12.52	15.57	15.36	14.77	15.05	18.59
SiH3 (Silyl)	8.74	8.84	5.76	5.37	5.43	6.15	8.80	8.60	8.16	7.24	8.93
SiH4 (Silane)	12.30	12.86	9.00	8.52	8.86	9.67	12.66	12.37	11.82	11.10	13.12
SiO (Silicon monoxide)[7]	11.61	11.51	8.06	7.47	7.57	8.61	11.43	11.23	10.74	10.10	12.34
SO2 (Sulfur dioxide)	12.50	12.58	8.71	8.03	8.07	9.39	12.29	12.07	11.53	11.12	13.92
MAE[a]			3.86	4.44	4.29	3.19	0.42	0.55	1.06	1.51	0.99
MSE[a]			-3.86	-4.44	-4.29	-3.19	-0.28	-0.53	-1.06	-1.51	0.89
RMS[a]			3.98	4.55	4.39	3.27	0.67	0.80	1.24	1.59	1.15
MAE[b]			3.92	4.50	4.35	3.25	0.41	0.59	1.13	1.57	0.91
MSE[b]			-3.92	-4.50	-4.35	-3.25	-0.34	-0.59	-1.12	-1.57	0.84
RMS[b]			4.05	4.61	4.45	3.32	0.67	0.82	1.28	1.63	1.04

[a] The reference values are experimental data.

[b] The reference values are calculated by CCSD.

Table S3. Vertical electron affinities (1) [in eV] of the 121 molecules studied. The reference values are calculated by CCSD.

Molecule	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	0.38	1.02	0.59	0.33	0.46	0.20	0.28	0.38	0.31	0.34
AlCl3 (Aluminum trichloride)	0.02	0.85	0.31	-0.33	0.24	-0.29	-0.17	-0.08	0.10	0.59
Ar (Argon atom)	-2.81	-2.05	-2.59	-3.14	-2.57	-2.94	-2.88	-2.73	-2.54	-2.19
B (Boron atom)	0.18	1.13	0.62	0.26	0.46	0.12	0.24	0.35	0.25	0.14
BCl3 (Borane, trichloro-)	-0.25	0.48	-0.02	-0.25	-0.07	-0.17	-0.13	-0.13	-0.10	0.12
Be (Beryllium atom)	-0.38	0.37	0.01	-0.21	-0.07	-0.43	-0.35	-0.24	-0.30	-0.37
BF3 (Borane, trifluoro-)	-1.04	-0.15	-0.60	-0.82	-0.62	-1.12	-1.01	-0.97	-0.84	-0.42
C (Carbon atom)	1.16	2.22	1.59	1.29	1.37	1.14	1.23	1.31	1.26	1.12
C2F4 (Tetrafluoroethylene)	-1.21	-0.32	-0.78	-1.66	-0.81	-1.32	-1.29	-1.21	-1.10	-1.30
C2H2 (Acetylene)	-2.01	-0.09	-0.37	-0.47	-0.43	-0.71	-0.70	-0.65	-0.64	-1.89
C2H2O2 (Ethanedial)	0.63	1.71	1.05	0.79	1.06	0.83	0.89	0.91	0.95	1.13
C2H4 (Ethylene)	-1.82	-0.12	-0.46	-0.69	-0.63	-0.75	-0.73	-0.86	-0.81	-1.70
C2H4O (Ethylene oxide)	-0.87	-0.04	-0.39	-0.70	-0.43	-0.68	-0.67	-0.61	-0.77	-0.73
C2H4S (Thiirane)	-0.79	-0.10	-0.44	-0.69	-0.51	-0.69	-0.67	-0.61	-0.74	-0.64
C2H5N (Aziridine)	-0.56	0.00	-0.36	-0.64	-0.41	-0.65	-0.63	-0.56	-0.57	-0.22
C2H6 (Ethane)	-0.63	-0.06	-0.42	-0.78	-0.47	-0.72	-0.71	-0.66	-0.60	-0.24
C2HF3 (Trifluoroethylene)	-0.56	0.02	-0.35	-1.57	-0.40	-0.66	-0.64	-0.57	-1.58	-1.47
C2N2 (Cyanogen)	-0.22	0.80	0.16	-0.08	0.22	0.06	0.11	0.12	0.10	0.32
C3H4 (Cyclopropene)	-1.76	-0.11	-0.43	-1.54	-0.51	-0.72	-0.70	-0.64	-0.60	-1.60
C3H6 (Cyclopropane)	-0.66	-0.08	-0.43	-0.72	-0.49	-0.77	-0.75	-0.70	-0.61	-0.25
C3H8 (Propane)	-0.61	-0.02	-0.38	-0.69	-0.44	-0.73	-0.71	-0.66	-0.55	-0.16
C3O2 (Carbon suboxide)	-0.66	-0.11	-0.75	-1.01	-0.57	-1.00	-0.97	-0.91	-0.77	-0.07
C4H2 (Diacetylene)	-1.24	-0.13	-0.65	-1.00	-0.72	-0.66	-0.65	-0.99	-0.97	-0.89
C4H4O (Furan)	-0.74	-0.01	-0.35	-0.62	-0.41	-0.67	-0.65	-0.60	-1.49	-1.45
C4H6 (Cyclobutene)	-2.30	-0.04	-0.39	-0.95	-0.45	-0.72	-0.71	-0.65	-1.16	-2.24
C4N2 (2-Butynedinitrile)	0.64	1.76	1.08	0.87	1.11	0.95	0.99	1.01	1.01	1.23
CCl4 (Carbon tetrachloride)	-0.39	0.77	0.24	-0.04	0.10	-0.48	-0.39	-0.25	-0.26	-0.45
CF2Cl2 (Difluorodichloromethane)	-0.89	0.04	-0.43	-0.83	-0.52	-1.14	-1.06	-0.92	-0.87	-0.58
CF2O (Carbonic difluoride)	-2.39	-0.30	-0.76	-1.36	-0.78	-1.25	-1.21	-1.14	-1.48	-1.48
CF3Br (Bromotrifluoromethane)	-0.79	0.03	-0.46	-0.80	-0.49	-0.95	-0.87	-0.75	-0.74	-0.54
CF3Cl (Methane, chlorotrifluoro-)	-1.05	-0.31	-0.74	-1.23	-0.81	-1.22	-1.17	-1.08	-1.06	-0.69
CF4 (Carbon tetrafluoride)	-1.34	-0.59	-1.02	-1.72	-1.07	-1.53	-1.52	-1.47	-1.30	-0.86
CFCl3 (Trichloromonofluoromethane)	-0.62	0.44	-0.07	-0.46	-0.17	-0.77	-0.68	-0.55	-0.56	-0.70
CH2CCH2 (Allene)	-0.57	-0.02	-0.37	-0.76	-0.42	-0.67	-0.66	-0.62	-0.91	-0.18
CH2CCl2 (Ethene, 1,1-dichloro-)	-0.97	-0.21	-0.34	-1.05	-0.41	-0.67	-0.65	-0.59	-0.57	-0.20

CH2CF2 (Ethene, 1,1-difluoro-)	-0.97	-0.01	-0.37	-0.60	-0.42	-0.67	-0.65	-0.60	-0.57	-1.50
CH2CHCHO (Acrolein)	-0.46	0.68	0.06	-0.20	0.03	-0.15	-0.11	-0.10	-0.06	0.05
CH2CHCl (Ethene, chloro-)	-0.86	-0.54	-0.39	-1.30	-0.44	-0.67	-0.65	-0.58	-1.31	-1.30
CH2CHF (Ethene, fluoro-)	-0.87	-0.08	-0.42	-1.54	-1.37	-0.69	-0.67	-0.61	-1.65	-1.71
CH2Cl2 (Methylene chloride)	-0.51	0.13	-0.29	-0.65	-0.35	-0.64	-0.61	-0.54	-0.55	-0.23
CH2CO (Ketene)	-0.52	-0.01	-0.40	-0.62	-0.37	-0.63	-0.61	-0.55	-0.81	-0.80
CH2F2 (Methane, difluoro-)	-0.59	-0.04	-0.38	-0.66	-0.42	-0.65	-0.63	-0.57	-0.61	-0.33
CH3 (Methyl radical)	-0.23	0.82	0.06	-0.22	0.01	-0.22	-0.15	-0.10	-0.09	0.03
CH3CCCH3 (2-Butyne)	-0.68	0.06	-0.30	-0.54	-0.93	-0.67	-0.66	-0.61	-0.60	-0.63
CH3CCH (Propyne)	-0.55	0.01	-0.35	-0.64	-0.41	-0.64	-0.62	-0.56	-0.52	-0.54
CH3CH2Cl (Ethyl chloride)	-0.52	0.06	-0.32	-0.77	-0.37	-0.63	-0.60	-0.54	-0.54	-0.16
CH3CH2OH (Ethanol)	-0.54	0.07	-0.31	-0.66	-0.36	-0.64	-0.62	-0.55	-0.53	-0.17
CH3Cl (Methyl chloride)	-0.52	0.06	-0.32	-0.58	-0.37	-0.62	-0.59	-0.53	-0.55	-1.14
CH3COCl (Acetyl Chloride)	-0.91	0.19	-0.25	-0.51	-0.27	-0.55	-0.53	-0.47	-0.70	-0.69
CH3F (Methyl fluoride)	-0.59	-0.05	-0.39	-0.61	-0.43	-0.65	-0.63	-0.58	-0.60	-0.32
CH3NHCH3 (Dimethylamine)	-0.56	0.03	-0.34	-0.62	-0.40	-0.68	-0.67	-0.60	-0.52	-0.32
CH3NO2 (Methane, nitro-)	-0.28	0.56	0.07	-0.18	0.06	-0.49	-0.47	-0.41	-0.16	0.18
CH3OCH3 (Dimethyl ether)	-0.59	0.00	-0.36	-0.67	-0.41	-0.69	-0.68	-0.62	-0.55	-0.19
CH3OH (Methyl alcohol)	-0.55	0.03	-0.34	-0.58	-0.38	-0.64	-0.62	-0.55	-0.56	-0.27
CH3SH (Methanethiol)	-0.52	0.09	-0.31	-0.69	-0.36	-0.64	-0.62	-0.56	-0.53	-0.21
CH3SiH3 (Methyl silane)	-0.53	0.05	-0.32	-0.57	-0.37	-0.64	-0.63	-0.57	-0.49	-0.14
CH4 (Methane)	-0.63	-0.09	-0.44	-0.74	-0.48	-0.68	-0.67	-0.62	-0.61	-0.32
CHCl3 (Chloroform)	-0.55	0.27	-0.22	-0.54	-0.33	-0.69	-0.65	-0.57	-0.56	-0.24
CHF3 (Methane, trifluoro-)	-0.61	-0.07	-0.42	-0.69	-0.46	-0.68	-0.65	-0.59	-0.60	-0.36
CHONH2 (Formamide)	-0.36	0.19	-0.18	-1.55	-0.22	-0.44	-0.41	-0.34	-1.61	-1.54
Cl (Chlorine atom)	3.51	3.97	3.65	3.59	3.67	3.56	3.62	3.66	3.61	3.65
Cl2 (Chlorine diatomic)	0.64	1.45	0.89	0.61	0.90	0.69	0.73	0.75	0.70	0.79
ClF (Chlorine monofluoride)	0.34	1.21	0.62	0.32	0.65	0.44	0.46	0.46	0.39	0.47
ClF3 (Chlorine trifluoride)	1.19	1.69	1.05	0.83	1.29	1.18	1.18	1.14	1.23	1.60
ClO (Monochlorine monoxide)	2.04	2.31	1.95	1.80	2.07	2.06	2.05	2.03	2.16	2.38
CO (Carbon monoxide)	-1.49	-0.48	-0.91	-1.18	-0.99	-1.53	-1.50	-1.25	-1.32	-1.41
CO2 (Carbon dioxide)	-0.84	-0.18	-0.65	-1.37	-0.65	-1.06	-1.02	-0.95	-0.87	-0.59
CS (Carbon monosulfide)	-0.08	0.61	0.10	-0.12	0.16	-1.14	-1.10	0.09	-0.01	0.13
CS2 (Carbon disulfide)	0.07	0.54	0.03	-0.22	0.14	-1.23	0.19	0.14	0.07	0.37
F (Fluorine atom)	3.21	4.63	3.65	3.08	3.53	3.44	3.38	3.34	3.27	3.37
F2 (Fluorine diatomic)	0.42	1.32	0.67	0.35	0.81	0.62	0.61	0.58	0.54	0.68
F2O (Difluorine monoxide)	-0.38	0.55	-0.08	-0.45	0.04	-0.24	-0.23	-0.24	-0.32	-0.19
FCN (Cyanogen fluoride)	-0.69	0.07	-0.42	-1.06	-0.44	-0.87	-0.82	-0.74	-0.68	-0.43

H (Hydrogen atom)	0.74	1.31	0.71	0.59	0.91	0.65	0.74	0.81	0.61	0.65
H2CO (Formaldehyde)	-0.55	0.01	-0.49	-0.81	-0.40	-1.01	-0.59	-0.83	-0.82	-0.79
H2CS (Thioformaldehyde)	0.26	0.95	0.42	0.24	0.46	0.42	0.43	0.41	0.37	0.43
H2O (Water)	-0.58	0.02	-0.38	-0.80	-0.40	-0.69	-0.66	-0.59	-0.59	-0.38
H2O2 (Hydrogen peroxide)	-0.92	-0.01	-0.41	-0.78	-0.55	-0.79	-0.75	-0.68	-0.85	-0.84
H2S (Hydrogen sulfide)	-0.50	0.08	-0.32	-0.73	-0.36	-0.63	-0.60	-0.53	-0.56	-0.34
HCCCN (Cyanoacetylene)	-0.36	0.36	-0.20	-0.48	-0.24	-0.53	-0.40	-0.44	-0.45	-0.30
HCCF (Fluoroacetylene)	-0.56	0.02	-0.35	-1.71	-0.39	-0.64	-0.62	-0.56	-1.71	-1.64
HCl (Hydrogen sulfide)	-0.52	0.07	-0.33	-0.69	-0.36	-0.65	-0.60	-0.53	-0.59	-0.43
HCN (Hydrogen cyanide)	-0.49	0.00	-0.34	-1.31	-0.37	-0.52	-0.49	-0.43	-1.43	-1.50
HCO (Formyl radical)	-0.05	0.69	0.06	-0.06	0.14	-0.06	0.00	0.03	0.09	0.25
HCOOH (Formic acid)	-0.59	0.01	-0.35	-1.35	-0.39	-0.68	-0.64	-0.57	-1.46	-1.54
He (Helium atom)	-2.63	-2.05	-2.32	-2.63	-2.37	-2.64	-2.60	-2.49	-2.47	-2.26
HF (Hydrogen fluoride)	-0.64	-0.05	-0.44	-0.84	-0.45	-0.73	-0.69	-0.61	-0.65	-0.46
Li (Lithium atom)	0.62	0.93	0.51	0.52	0.56	0.40	0.48	0.51	0.52	0.40
Mg (Magnesium atom)	-0.24	0.30	-0.02	-0.20	-0.08	-0.33	-0.29	-0.22	-0.26	-0.24
N (Nitrogen atom)	-0.34	0.81	0.28	-0.21	0.23	-0.08	-0.08	-0.08	-0.14	-0.01
N2 (Nitrogen diatomic)	-2.32	-1.16	-1.64	-1.92	-1.45	-1.91	-1.86	-1.75	-1.70	-2.05
N2H4 (Hydrazine)	-0.46	0.15	-0.26	-0.69	-0.30	-0.58	-0.54	-0.48	-0.48	-0.27
N2O (Nitrous oxide)	-2.05	-0.53	-0.97	-2.03	-1.00	-1.48	-1.43	-1.35	-1.85	-1.56
Na (Sodium atom)	0.54	0.96	0.55	0.47	0.58	0.54	0.57	0.52	0.56	0.53
NaCl (Sodium Chloride)	0.64	1.19	0.80	0.37	0.82	0.57	0.59	0.65	0.62	1.01
Ne (Neon atom)	-5.32	-4.41	-4.93	-5.46	-4.90	-5.57	-5.43	-5.32	-4.89	-4.58
NF3 (Nitrogen trifluoride)	-2.04	-0.92	-1.37	-2.03	-1.43	-1.96	-1.93	-1.85	-1.67	-1.25
NH (Imidogen)	0.14	1.29	0.56	0.22	0.51	0.29	0.32	0.32	0.27	0.24
NH2 (Amino radical)	0.54	1.67	0.84	0.45	0.76	0.61	0.64	0.66	0.69	0.90
NH3 (Ammonia)	-0.57	0.00	-0.38	-0.77	-0.41	-0.67	-0.65	-0.58	-0.60	-0.35
NO (Nitric oxide)	-0.43	0.19	-0.13	-0.41	-0.06	-0.28	-0.24	-0.22	-0.24	-0.09
NO2 (Nitrogen dioxide)	1.47	1.92	1.20	0.84	1.45	1.39	1.41	1.36	1.54	2.15
O (Oxygen atom)	1.24	2.57	1.78	1.26	1.68	1.48	1.48	1.46	1.41	1.34
O2 (Oxygen diatomic)	-0.14	0.60	-0.11	-0.44	0.05	-0.12	-0.08	-0.10	-0.03	0.34
O3 (Ozone)	2.30	2.56	1.91	1.83	2.44	2.48	2.49	2.41	2.68	3.30
OCS (Carbonyl sulfide)	-0.86	-0.51	-1.00	-1.31	-0.70	-1.05	-1.00	-0.92	-1.20	-0.92
OH (Hydroxyl radical)	1.60	2.86	1.97	1.49	1.85	1.73	1.73	1.71	1.70	1.90
P (Phosphorus atom)	0.61	1.50	0.88	0.61	0.96	0.72	0.82	0.88	0.86	0.96
P2 (Phosphorus diatomic)	0.46	1.07	0.58	0.42	0.62	0.66	0.66	0.64	0.53	0.71
PF3 (Phosphorus trifluoride)	-1.23	-0.42	-0.82	-1.20	-0.89	-1.37	-1.32	-1.21	-1.14	-1.01
PH3 (Phosphine)	-0.52	0.04	-0.34	-0.73	-0.39	-0.64	-0.61	-0.55	-0.57	-0.32

S (Sulfur atom)	1.95	2.87	2.17	1.99	2.20	2.03	2.12	2.16	2.11	2.19
S2 (Sulfur diatomic)	1.45	2.00	1.36	1.26	1.47	1.50	1.52	1.51	1.51	1.72
Si (Silicon atom)	1.34	1.63	1.49	1.39	1.34	1.19	1.24	1.32	1.26	1.23
Si2H6 (Disilane)	-0.66	0.04	-0.31	-0.84	-0.39	-0.69	-0.68	-0.62	-0.62	-0.55
SiF2 (Silicon difluoride)	0.07	0.75	0.29	0.05	0.29	0.08	0.13	0.17	0.13	0.24
SiF4 (Silicon tetrafluoride)	-0.81	0.04	-0.47	-1.31	-0.51	-1.03	-1.00	-0.94	-0.79	-0.36
SiH3 (Silyl)	0.82	1.61	0.94	0.74	0.97	0.81	0.88	0.92	0.83	0.96
SiH4 (Silane)	-0.59	-0.02	-0.38	-0.86	-0.43	-0.68	-0.66	-0.61	-0.58	-0.29
SiO (Silicon monoxide)	0.01	0.66	0.22	-0.02	0.22	-0.01	0.05	0.11	0.04	0.13
SO2 (Sulfur dioxide)	0.87	1.36	0.77	0.58	1.00	0.98	0.98	0.94	0.99	1.40
MAE		0.79	0.34	0.24	0.31	0.20	0.18	0.16	0.21	0.33
MSE		0.78	0.32	-0.07	0.30	0.02	0.07	0.13	0.05	0.17
RMS		0.86	0.46	0.38	0.43	0.34	0.32	0.31	0.37	0.42

Table S4. Vertical electron affinities (2) [in eV] of the 121 molecules studied. The reference values are calculated by CCSD.

Molecule	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	0.38	-0.86	-1.26	-1.56	-0.92	0.61	0.57	0.46	-0.44	0.44
AlCl3 (Aluminum trichloride)	0.02	-0.92	-1.39	-1.94	-1.08	-0.17	-0.05	-0.06	-0.65	0.61
Ar (Argon atom)	-2.81	-4.14	-4.59	-4.89	-4.31	-2.89	-2.81	-2.71	-3.40	-2.25
B (Boron atom)	0.18	-1.35	-1.77	-1.85	-1.32	0.56	0.51	0.30	-0.67	0.52
BCl3 (Borane, trichloro-)	-0.25	-2.09	-2.07	-2.22	-2.01	0.22	0.09	-0.31	-1.19	0.45
Be (Beryllium atom)	-0.38	-1.02	-1.31	-1.38	-1.14	-0.40	-0.31	-0.28	-0.91	-0.48
BF3 (Borane, trifluoro-)	-1.04	-1.64	-2.05	-1.86	-1.84	-1.10	-0.95	-0.93	-1.45	-0.68
C (Carbon atom)	1.16	-1.38	-1.88	-2.16	-1.15	1.36	1.21	0.83	-0.02	1.81
C2F4 (Tetrafluoroethylene)	-1.21	-1.71	-1.80	-2.77	-1.94	-1.28	-1.24	-1.17	-1.63	-1.58
C2H2 (Acetylene)	-2.01	-0.95	-1.25	-1.30	-1.16	-0.67	-0.65	-0.61	-1.12	-2.00
C2H2O2 (Ethanedial)	0.63	-1.63	-2.20	-2.36	-1.37	1.04	0.89	0.48	-0.21	1.63
C2H4 (Ethylene)	-1.82	-1.13	-1.45	-1.51	-1.36	-0.70	-0.68	-0.83	-1.27	-1.68
C2H4O (Ethylene oxide)	-0.87	-1.10	-1.42	-1.56	-1.30	-0.63	-0.61	-0.56	-1.24	-0.95
C2H4S (Thiirane)	-0.79	-1.16	-1.44	-1.60	-1.33	-0.62	-0.59	-0.54	-1.19	-0.88
C2H5N (Aziridine)	-0.56	-1.11	-1.43	-1.57	-1.31	-0.59	-0.55	-0.51	-1.11	-0.41
C2H6 (Ethane)	-0.63	-1.10	-1.44	-1.65	-1.32	-0.68	-0.66	-0.62	-1.14	-0.45
C2HF3 (Trifluoroethylene)	-0.56	-1.12	-1.47	-2.89	-1.33	-0.60	-0.57	-0.53	-2.30	-1.69
C2N2 (Cyanogen)	-0.22	-2.54	-3.09	-3.26	-2.24	0.17	0.01	-0.39	-1.17	0.72
C3H4 (Cyclopropene)	-1.76	-1.05	-1.37	-2.86	-1.24	-0.67	-0.65	-0.60	-1.17	-1.56
C3H6 (Cyclopropane)	-0.66	-1.08	-1.41	-1.61	-1.31	-0.72	-0.71	-0.66	-1.15	-0.46
C3H8 (Propane)	-0.61	-1.01	-1.35	-1.52	-1.25	-0.68	-0.66	-0.62	-1.09	-0.33
C3O2 (Carbon suboxide)	-0.66	-3.43	-3.86	-4.17	-3.00	-0.95	-0.91	-0.85	-1.33	0.37
C4H2 (Diacetylene)	-1.24	-2.15	-2.44	-2.58	-2.19	-0.62	-0.60	-1.13	-1.81	-0.79
C4H4O (Furan)	-0.74	-0.93	-1.26	-1.48	-1.17	-0.62	-0.59	-0.55	-2.13	-1.68
C4H6 (Cyclobutene)	-2.30	-1.00	-1.33	-1.71	-1.23	-0.67	-0.65	-0.61	-1.58	-2.03
C4N2 (2-Butynedinitrile)	0.64	-1.14	-1.74	-1.87	-1.03	1.19	1.05	0.70	-0.09	1.57
CCl4 (Carbon tetrachloride)	-0.39	-1.49	-1.89	-2.52	-1.52	-0.16	-0.21	-0.34	-1.08	-0.10
CF2Cl2 (Difluorodichloromethane)	-0.89	-1.67	-2.02	-2.29	-1.80	-1.07	-0.99	-0.93	-1.51	-0.77
CF2O (Carbonic difluoride)	-2.39	-1.86	-2.28	-2.65	-2.06	-1.19	-1.13	-1.09	-2.16	-1.70
CF3Br (Bromotrifluoromethane)	-0.79	-1.87	-2.17	-2.58	-2.01	-0.84	-0.79	-0.80	-1.65	-0.35
CF3Cl (Methane, chlorotrifluoro-)	-1.05	-1.77	-2.14	-2.60	-1.96	-1.11	-1.06	-1.05	-1.70	-0.89
CF4 (Carbon tetrafluoride)	-1.34	-1.98	-2.39	-2.85	-2.22	-1.47	-1.44	-1.41	-1.94	-1.22
CFCl3 (Trichloromonofluoromethane)	-0.62	-1.62	-2.00	-2.44	-1.69	-0.53	-0.56	-0.66	-1.37	-0.29
CH2CCH2 (Allene)	-0.57	-0.99	-1.32	-1.69	-1.22	-0.63	-0.61	-0.58	-1.43	-0.39
CH2CCl2 (Ethene, 1,1-dichloro-)	-0.97	-2.20	-1.43	-2.76	-1.29	-0.59	-0.56	-0.52	-1.11	-0.44

CH2CF2 (Ethene, 1,1-difluoro-)	-0.97	-1.09	-1.43	-1.55	-1.31	-0.61	-0.59	-0.55	-1.13	-1.73
CH2CHCHO (Acrolein)	-0.46	-2.20	-2.67	-3.00	-2.08	0.15	0.00	-0.37	-1.13	0.40
CH2CHCl (Ethene, chloro-)	-0.86	-2.47	-1.44	-2.92	-1.32	-0.59	-0.57	-0.53	-2.12	-1.12
CH2CHF (Ethene, fluoro-)	-0.87	-1.13	-1.45	-3.02	-2.70	-0.63	-0.61	-0.57	-2.46	-1.68
CH2Cl2 (Methylene chloride)	-0.51	-1.27	-1.60	-1.82	-1.41	-0.55	-0.52	-0.47	-1.11	-0.47
CH2CO (Ketene)	-0.52	-1.46	-1.71	-1.83	-1.27	-0.57	-0.54	-0.50	-1.36	-0.89
CH2F2 (Methane, difluoro-)	-0.59	-1.18	-1.51	-1.72	-1.37	-0.60	-0.58	-0.54	-1.22	-0.57
CH3 (Methyl radical)	-0.23	-1.89	-2.37	-2.31	-1.77	0.46	0.33	0.03	-0.90	0.57
CH3CCCH3 (2-Butyne)	-0.68	-0.89	-1.24	-1.27	-1.60	-0.62	-0.61	-0.57	-1.04	-0.56
CH3CCH (Propyne)	-0.55	-1.02	-1.32	-1.63	-1.13	-0.57	-0.55	-0.50	-0.92	-0.59
CH3CH2Cl (Ethyl chloride)	-0.52	-1.08	-1.43	-1.74	-1.30	-0.56	-0.52	-0.49	-1.07	-0.36
CH3CH2OH (Ethanol)	-0.54	-1.05	-1.39	-1.54	-1.26	-0.58	-0.55	-0.50	-1.06	-0.34
CH3Cl (Methyl chloride)	-0.52	-1.17	-1.51	-1.50	-1.36	-0.56	-0.52	-0.47	-1.11	-1.33
CH3COCl (Acetyl Chloride)	-0.91	-1.43	-1.70	-1.87	-1.22	-0.48	-0.45	-0.40	-1.34	-0.01
CH3F (Methyl fluoride)	-0.59	-1.16	-1.49	-1.53	-1.36	-0.60	-0.58	-0.54	-1.19	-0.55
CH3NHCH3 (Dimethylamine)	-0.56	-1.01	-1.34	-1.47	-1.23	-0.63	-0.61	-0.56	-1.03	-0.11
CH3NO2 (Methane, nitro-)	-0.28	-1.45	-1.71	-1.88	-1.53	-0.42	-0.39	-0.35	-1.12	1.43
CH3OCH3 (Dimethyl ether)	-0.59	-1.02	-1.35	-1.50	-1.25	-0.65	-0.62	-0.57	-1.07	-0.38
CH3OH (Methyl alcohol)	-0.55	-1.13	-1.46	-1.49	-1.33	-0.59	-0.56	-0.51	-1.10	-0.49
CH3SH (Methanethiol)	-0.52	-1.09	-1.44	-1.60	-1.30	-0.58	-0.55	-0.50	-1.03	-0.44
CH3SiH3 (Methyl silane)	-0.53	-1.01	-1.26	-1.38	-1.16	-0.60	-0.58	-0.53	-1.00	-0.37
CH4 (Methane)	-0.63	-1.17	-1.49	-1.76	-1.37	-0.63	-0.61	-0.58	-1.16	-0.59
CHCl3 (Chloroform)	-0.55	-1.49	-1.87	-2.06	-1.63	-0.58	-0.54	-0.50	-1.24	-0.51
CHF3 (Methane, trifluoro-)	-0.61	-1.26	-1.59	-1.77	-1.45	-0.62	-0.60	-0.57	-1.19	-0.57
CHONH2 (Formamide)	-0.36	-1.07	-1.41	-2.77	-1.24	-0.36	-0.33	-0.29	-2.27	-1.73
Cl (Chlorine atom)	3.51	0.03	-0.24	-0.15	0.79	3.70	3.45	2.92	2.23	4.27
Cl2 (Chlorine diatomic)	0.64	-1.51	-1.98	-2.38	-1.37	0.83	0.65	0.28	-0.45	1.27
ClF (Chlorine monofluoride)	0.34	-2.14	-2.63	-3.02	-1.90	0.41	0.24	-0.17	-0.89	0.95
ClF3 (Chlorine trifluoride)	1.19	-1.90	-2.40	-2.71	-1.40	1.23	1.01	0.50	-0.01	2.47
ClO (Monochlorine monoxide)	2.04	-1.50	-1.82	-1.83	-0.63	2.20	1.98	1.45	1.03	3.56
CO (Carbon monoxide)	-1.49	-2.46	-2.74	-2.83	-2.49	-1.45	-1.41	-1.38	-2.19	-1.44
CO2 (Carbon dioxide)	-0.84	-1.75	-2.15	-2.58	-1.93	-1.02	-0.96	-0.91	-1.50	-0.77
CS (Carbon monosulfide)	-0.08	-2.41	-2.82	-3.10	-2.12	-1.04	-1.00	-0.30	-1.18	0.67
CS2 (Carbon disulfide)	0.07	-2.01	-2.41	-2.85	-1.79	-1.18	0.31	-0.07	-0.93	0.86
F (Fluorine atom)	3.21	-0.88	-1.53	-1.54	-0.03	3.08	2.84	2.20	2.06	5.19
F2 (Fluorine diatomic)	0.42	-3.04	-3.50	-3.62	-2.48	0.12	-0.05	-0.56	-0.67	2.46
F2O (Difluorine monoxide)	-0.38	-3.12	-3.56	-4.09	-2.75	-0.38	-0.55	-1.02	-1.50	1.18
FCN (Cyanogen fluoride)	-0.69	-1.72	-2.15	-2.33	-1.87	-0.80	-0.73	-0.72	-1.40	-0.59

H (Hydrogen atom)	0.74	-1.23	-1.71	-1.32	-1.00	1.40	1.32	0.99	-0.14	1.42
H2CO (Formaldehyde)	-0.55	-2.35	-2.64	-2.73	-1.36	-0.96	-0.52	-1.11	-1.81	-0.59
H2CS (Thioformaldehyde)	0.26	-2.08	-2.52	-2.78	-1.79	0.66	0.48	0.06	-0.79	0.79
H2O (Water)	-0.58	-1.40	-1.75	-1.85	-1.57	-0.64	-0.59	-0.54	-1.26	-0.75
H2O2 (Hydrogen peroxide)	-0.92	-1.36	-1.72	-1.87	-1.57	-0.74	-0.69	-0.64	-1.39	-1.12
H2S (Hydrogen sulfide)	-0.50	-1.17	-1.51	-1.72	-1.37	-0.58	-0.54	-0.48	-1.06	-0.56
HCCCN (Cyanoacetylene)	-0.36	-2.04	-2.34	-2.45	-2.04	-0.36	-0.31	-0.73	-1.49	-0.08
HCCF (Fluoroacetylene)	-0.56	-1.07	-1.40	-2.90	-1.28	-0.59	-0.57	-0.52	-2.38	-1.85
HCl (Hydrogen sulfide)	-0.52	-1.32	-1.67	-1.88	-1.49	-0.60	-0.54	-0.49	-1.25	-0.71
HCN (Hydrogen cyanide)	-0.49	-1.26	-1.58	-2.73	-1.42	-0.46	-0.42	-0.40	-2.19	-1.73
HCO (Formyl radical)	-0.05	-2.22	-2.60	-2.59	-1.98	0.30	0.19	-0.15	-0.94	0.91
HCOOH (Formic acid)	-0.59	-1.12	-1.43	-2.71	-1.31	-0.61	-0.57	-0.53	-2.18	-1.48
He (Helium atom)	-2.63	-3.93	-4.19	-4.33	-3.92	-2.63	-2.56	-2.52	-3.65	-3.02
HF (Hydrogen fluoride)	-0.64	-1.64	-2.00	-2.11	-1.77	-0.69	-0.64	-0.61	-1.45	-0.86
Li (Lithium atom)	0.62	-0.51	-0.86	-0.94	-0.57	0.69	0.72	0.70	-0.10	0.47
Mg (Magnesium atom)	-0.24	-0.66	-0.92	-0.93	-0.80	-0.32	-0.27	-0.20	-0.71	-0.39
N (Nitrogen atom)	-0.34	-2.67	-3.09	-3.14	-2.30	0.18	0.00	-0.45	-1.43	0.16
N2 (Nitrogen diatomic)	-2.32	-3.74	-3.98	-4.01	-2.45	-1.86	-1.81	-1.71	-2.30	-1.55
N2H4 (Hydrazine)	-0.46	-1.20	-1.57	-1.80	-1.39	-0.51	-0.47	-0.44	-1.11	-0.38
N2O (Nitrous oxide)	-2.05	-2.03	-2.40	-4.02	-2.20	-1.42	-1.35	-1.29	-2.83	-0.87
Na (Sodium atom)	0.54	-0.49	-0.83	-0.83	-0.55	0.69	0.69	0.66	-0.09	0.45
NaCl (Sodium Chloride)	0.64	-0.46	-0.80	-0.88	-0.51	0.63	0.66	0.67	-0.12	0.75
Ne (Neon atom)	-5.32	-7.28	-7.68	-7.81	-7.27	-5.43	-5.39	-5.53	-6.25	-5.03
NF3 (Nitrogen trifluoride)	-2.04	-2.59	-2.98	-3.37	-2.71	-1.89	-1.84	-1.79	-2.30	-1.59
NH (Imidogen)	0.14	-2.27	-2.79	-2.84	-1.94	0.68	0.50	0.03	-0.78	1.29
NH2 (Amino radical)	0.54	-1.89	-2.47	-2.49	-1.57	1.14	0.94	0.47	-0.26	1.86
NH3 (Ammonia)	-0.57	-1.27	-1.60	-1.83	-1.45	-0.62	-0.59	-0.53	-1.17	-0.65
NO (Nitric oxide)	-0.43	-3.43	-3.71	-3.86	-2.85	-0.32	-0.51	-0.95	-1.55	0.98
NO2 (Nitrogen dioxide)	1.47	-1.59	-2.16	-2.58	-1.13	1.55	1.36	0.84	0.37	3.16
O (Oxygen atom)	1.24	-1.93	-2.47	-2.63	-1.32	1.60	1.38	0.80	0.26	2.82
O2 (Oxygen diatomic)	-0.14	-3.62	-4.16	-4.48	-2.97	-0.19	-0.40	-0.95	-1.34	1.74
O3 (Ozone)	2.30	-1.60	-2.15	-2.19	-0.57	2.40	2.17	1.56	1.44	4.24
OCS (Carbonyl sulfide)	-0.86	-2.75	-3.02	-3.19	-1.80	-0.93	-0.89	-0.86	-2.18	-0.41
OH (Hydroxyl radical)	1.60	-1.51	-2.13	-2.18	-0.94	2.03	1.80	1.23	0.76	3.46
P (Phosphorus atom)	0.61	-1.30	-1.77	-1.97	-1.11	1.02	0.95	0.67	-0.29	1.21
P2 (Phosphorus diatomic)	0.46	-1.64	-2.04	-2.28	-1.43	0.90	0.73	0.37	-0.58	1.03
PF3 (Phosphorus trifluoride)	-1.23	-1.86	-2.17	-2.38	-2.00	-1.33	-1.27	-1.20	-1.80	-1.17
PH3 (Phosphine)	-0.52	-1.09	-1.43	-1.71	-1.31	-0.60	-0.56	-0.51	-1.09	-0.55

S (Sulfur atom)	1.95	-0.58	-1.11	-1.22	-0.27	2.34	2.17	1.74	0.89	2.77
S2 (Sulfur diatomic)	1.45	-1.08	-1.62	-1.75	-0.79	1.75	1.56	1.15	0.34	2.25
Si (Silicon atom)	1.34	-0.98	-1.13	-1.28	-0.63	1.54	1.41	1.13	0.18	1.48
Si2H6 (Disilane)	-0.66	-0.89	-1.20	-1.72	-1.12	-0.65	-0.63	-0.58	-1.06	-0.81
SiF2 (Silicon difluoride)	0.07	-1.57	-1.93	-2.06	-1.54	0.24	0.15	-0.08	-0.94	0.22
SiF4 (Silicon tetrafluoride)	-0.81	-1.52	-1.98	-2.47	-1.75	-1.00	-0.94	-0.90	-1.28	-0.48
SiH3 (Silyl)	0.82	-0.97	-1.45	-1.63	-0.89	1.21	1.12	0.86	-0.05	1.43
SiH4 (Silane)	-0.59	-1.05	-1.37	-1.78	-1.26	-0.64	-0.61	-0.57	-1.15	-0.66
SiO (Silicon monoxide)	0.01	-1.54	-1.90	-1.98	-1.52	0.12	0.06	-0.13	-0.97	0.05
SO2 (Sulfur dioxide)	0.87	-2.12	-2.58	-2.84	-1.62	1.04	0.82	0.33	-0.34	2.02
MAE		1.31	1.67	1.95	1.28	0.24	0.20	0.24	0.80	0.55
MSE		-1.27	-1.62	-1.92	-1.22	0.13	0.12	0.00	-0.75	0.34
RMS		1.60	1.97	2.20	1.47	0.39	0.35	0.39	0.87	0.76

Table S5. Vertical electron affinities (3) [in eV] of the 121 molecules studied. The reference values are calculated by CCSD.

Molecule	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	0.38	3.32	2.76	2.29	2.11	-0.02	0.11	0.38	1.27	3.65
AlCl3 (Aluminum trichloride)	0.02	2.92	2.22	1.55	1.70	-0.41	-0.32	-0.13	1.00	0.79
Ar (Argon atom)	-2.81	-0.31	-0.65	-1.79	-0.92	-3.22	-3.31	-3.07	-1.72	-1.57
B (Boron atom)	0.18	4.36	3.62	2.74	2.68	-0.14	0.12	0.56	1.41	3.91
BCl3 (Borane, trichloro-)	-0.25	3.45	2.72	2.37	1.98	-0.69	-0.45	-0.04	0.92	0.32
Be (Beryllium atom)	-0.38	2.52	2.02	1.68	1.43	-0.50	-0.46	-0.24	0.53	0.27
BF3 (Borane, trifluoro-)	-1.04	1.21	0.78	0.33	0.51	-1.19	-1.29	-1.12	0.15	0.21
C (Carbon atom)	1.16	6.49	5.58	4.77	4.28	0.99	1.37	1.95	2.70	3.43
C2F4 (Tetrafluoroethylene)	-1.21	1.15	0.58	0.12	0.30	-1.45	-1.56	-1.39	-0.04	0.03
C2H2 (Acetylene)	-2.01	1.04	0.41	-0.01	0.05	-0.85	-0.92	-0.85	-0.05	0.18
C2H2O2 (Ethanedial)	0.63	5.21	4.44	4.04	3.59	0.67	0.94	1.40	2.18	0.74
C2H4 (Ethylene)	-1.82	1.79	1.12	0.73	0.37	-0.90	-0.99	-0.87	0.00	0.19
C2H4O (Ethylene oxide)	-0.87	0.66	0.40	0.19	0.24	-0.84	-0.93	-0.80	0.09	0.26
C2H4S (Thiirane)	-0.79	1.54	0.95	0.61	0.36	-0.86	-0.95	-0.81	0.11	0.27
C2H5N (Aziridine)	-0.56	0.88	0.55	0.27	0.33	-0.81	-0.90	-0.77	0.14	0.28
C2H6 (Ethane)	-0.63	0.71	0.42	0.15	0.25	-0.88	-0.96	-0.83	0.07	0.22
C2HF3 (Trifluoroethylene)	-0.56	1.54	0.77	0.35	0.37	-0.81	-0.89	-0.77	0.16	0.32
C2N2 (Cyanogen)	-0.22	4.29	3.55	3.15	2.77	0.00	0.25	0.69	1.45	0.17
C3H4 (Cyclopropene)	-1.76	1.79	1.11	0.67	0.35	-0.87	-0.96	-0.84	-0.01	0.18
C3H6 (Cyclopropane)	-0.66	0.62	0.33	0.09	0.16	-0.92	-1.00	-0.87	0.02	0.18
C3H8 (Propane)	-0.61	0.78	0.47	0.16	0.27	-0.88	-0.96	-0.83	0.10	0.24
C3O2 (Carbon suboxide)	-0.66	3.31	2.55	2.18	1.91	-0.70	-0.47	-0.08	0.78	0.23
C4H2 (Diacetylene)	-1.24	2.53	1.84	1.45	1.14	-0.76	-0.82	-0.75	0.09	0.25
C4H4O (Furan)	-0.74	1.56	0.88	0.55	0.20	-0.83	-0.91	-0.79	0.07	0.26
C4H6 (Cyclobutene)	-2.30	1.32	0.66	0.28	0.20	-0.88	-0.96	-0.84	0.06	0.23
C4N2 (2-Butynedinitrile)	0.64	4.72	3.97	3.62	3.29	0.74	0.97	1.35	2.15	0.99
CCl4 (Carbon tetrachloride)	-0.39	3.35	2.72	2.54	1.93	-0.77	-0.57	-0.15	0.67	0.16
CF2Cl2 (Difluorodichloromethane)	-0.89	2.60	1.92	1.61	1.18	-1.30	-1.26	-0.90	0.06	0.06
CF2O (Carbonic difluoride)	-2.39	2.62	1.77	1.21	0.92	-1.41	-1.50	-1.30	0.00	0.06
CF3Br (Bromotrifluoromethane)	-0.79	2.73	2.02	1.50	1.38	-1.15	-1.06	-0.71	0.29	0.07
CF3Cl (Methane, chlorotrifluoro-)	-1.05	1.98	1.27	0.83	0.58	-1.45	-1.51	-1.29	-0.16	-0.01
CF4 (Carbon tetrafluoride)	-1.34	0.48	0.19	-0.12	-0.04	-1.73	-1.86	-1.66	-0.30	-0.18
CFCl3 (Trichloromonofluoromethane)	-0.62	3.10	2.45	2.22	1.68	-1.01	-0.83	-0.41	0.45	0.11
CH2CCH2 (Allene)	-0.57	1.49	0.86	0.50	0.26	-0.83	-0.92	-0.79	0.09	0.25
CH2CCl2 (Ethene, 1,1-dichloro-)	-0.97	2.37	1.69	1.36	1.00	-0.85	-0.94	-0.81	0.12	0.31

CH2CF2 (Ethene, 1,1-difluoro-)	-0.97	1.47	0.76	0.30	0.31	-0.82	-0.91	-0.79	0.12	0.29
CH2CHCHO (Acrolein)	-0.46	3.80	3.07	2.72	2.27	-0.41	-0.19	0.21	1.08	0.39
CH2CHCl (Ethene, chloro-)	-0.86	2.13	1.45	1.10	0.72	-0.84	-0.93	-0.80	0.08	0.28
CH2CHF (Ethene, fluoro-)	-0.87	1.72	1.03	0.66	0.32	-0.85	-0.94	-0.82	0.05	0.26
CH2Cl2 (Methylene chloride)	-0.51	2.04	1.43	1.09	0.78	-0.82	-0.89	-0.74	0.24	0.35
CH2CO (Ketene)	-0.52	2.84	2.14	1.70	1.29	-0.78	-0.86	-0.73	0.17	0.34
CH2F2 (Methane, difluoro-)	-0.59	0.67	0.41	0.26	0.27	-0.80	-0.89	-0.77	0.12	0.30
CH3 (Methyl radical)	-0.23	4.07	2.95	2.25	2.19	-0.58	-0.36	0.00	1.23	3.04
CH3CCCH3 (2-Butyne)	-0.68	0.83	0.54	0.24	0.35	-0.81	-0.89	-0.76	0.15	0.30
CH3CCH (Propyne)	-0.55	0.78	0.50	0.23	0.33	-0.80	-0.88	-0.76	0.13	0.28
CH3CH2Cl (Ethyl chloride)	-0.52	1.14	0.68	0.34	0.40	-0.80	-0.88	-0.75	0.19	0.33
CH3CH2OH (Ethanol)	-0.54	1.00	0.66	0.33	0.42	-0.80	-0.88	-0.75	0.19	0.31
CH3Cl (Methyl chloride)	-0.52	1.35	0.88	0.52	0.51	-0.78	-0.86	-0.72	0.20	0.33
CH3COCl (Acetyl Chloride)	-0.91	3.04	2.33	1.91	1.49	-0.73	-0.80	-0.63	0.29	0.44
CH3F (Methyl fluoride)	-0.59	0.66	0.42	0.23	0.28	-0.80	-0.89	-0.77	0.11	0.28
CH3NHCH3 (Dimethylamine)	-0.56	0.89	0.56	0.24	0.33	-0.83	-0.91	-0.78	0.14	0.28
CH3NO2 (Methane, nitro-)	-0.28	3.92	3.17	2.84	2.42	-0.45	-0.22	0.22	0.97	0.50
CH3OCH3 (Dimethyl ether)	-0.59	0.82	0.50	0.21	0.31	-0.84	-0.93	-0.79	0.12	0.27
CH3OH (Methyl alcohol)	-0.55	1.01	0.67	0.35	0.43	-0.79	-0.87	-0.74	0.19	0.31
CH3SH (Methanethiol)	-0.52	1.26	0.84	0.45	0.53	-0.80	-0.88	-0.73	0.22	0.34
CH3SiH3 (Methyl silane)	-0.53	1.07	0.67	0.27	0.39	-0.78	-0.85	-0.73	0.15	0.30
CH4 (Methane)	-0.63	0.61	0.37	0.14	0.24	-0.85	-0.93	-0.80	0.05	0.21
CHCl3 (Chloroform)	-0.55	2.66	2.03	1.75	1.27	-0.89	-0.94	-0.72	0.25	0.32
CHF3 (Methane, trifluoro-)	-0.61	0.67	0.40	0.23	0.26	-0.83	-0.92	-0.80	0.10	0.27
CHONH2 (Formamide)	-0.36	1.51	0.82	0.49	0.61	-0.61	-0.70	-0.56	0.37	0.52
Cl (Chlorine atom)	3.51	8.11	7.73	7.32	6.76	3.64	4.00	4.56	5.09	3.31
Cl2 (Chlorine diatomic)	0.64	4.91	4.22	3.96	3.41	0.61	0.85	1.31	1.98	0.59
ClF (Chlorine monofluoride)	0.34	5.16	4.43	4.00	3.48	0.51	0.74	1.22	1.85	0.45
ClF3 (Chlorine trifluoride)	1.19	5.62	4.84	4.52	4.11	1.14	1.38	1.84	2.54	1.04
ClO (Monochlorine monoxide)	2.04	6.34	5.95	5.57	4.95	1.99	2.23	2.73	3.51	1.76
CO (Carbon monoxide)	-1.49	2.72	2.01	1.54	1.13	-1.57	-1.44	-1.04	-0.22	-0.38
CO2 (Carbon dioxide)	-0.84	1.33	0.90	0.33	0.60	-1.21	-1.27	-1.08	0.13	0.20
CS (Carbon monosulfide)	-0.08	4.06	3.40	3.12	2.62	-0.11	0.12	0.55	1.33	0.05
CS2 (Carbon disulfide)	0.07	3.46	2.83	2.60	2.23	-0.10	0.06	0.38	1.19	0.22
F (Fluorine atom)	3.21	10.80	9.30	7.66	7.55	4.05	4.22	4.80	4.74	2.21
F2 (Fluorine diatomic)	0.42	6.70	5.81	5.08	4.52	1.27	1.47	2.00	2.22	0.13
F2O (Difluorine monoxide)	-0.38	5.13	4.27	3.62	3.19	-0.06	0.18	0.70	1.11	-0.50
FCN (Cyanogen fluoride)	-0.69	2.07	1.53	0.82	1.05	-1.04	-1.07	-0.84	0.35	0.31

H (Hydrogen atom)	0.74	2.55	0.70	95.09	0.04	1.61	1.49	1.45	15.29	52.59
H2CO (Formaldehyde)	-0.55	3.41	2.69	2.25	1.78	-0.77	-0.85	-0.44	0.43	0.32
H2CS (Thioformaldehyde)	0.26	4.28	3.62	3.39	2.85	0.20	0.41	0.81	1.67	0.39
H2O (Water)	-0.58	1.24	0.93	0.49	0.68	-0.84	-0.92	-0.75	0.28	0.38
H2O2 (Hydrogen peroxide)	-0.92	2.40	1.68	0.96	0.73	-0.92	-1.02	-0.85	0.21	0.32
H2S (Hydrogen sulfide)	-0.50	1.21	0.84	0.36	0.58	-0.78	-0.84	-0.70	0.22	0.37
HCCCN (Cyanoacetylene)	-0.36	3.39	2.67	2.29	1.93	-0.59	-0.47	-0.08	0.75	0.46
HCCF (Fluoroacetylene)	-0.56	1.13	0.73	0.32	0.42	-0.79	-0.87	-0.75	0.12	0.27
HCl (Hydrogen sulfide)	-0.52	1.53	1.10	0.60	0.74	-0.78	-0.84	-0.69	0.25	0.36
HCN (Hydrogen cyanide)	-0.49	1.80	1.13	0.68	0.38	-0.67	-0.75	-0.65	0.14	0.36
HCO (Formyl radical)	-0.05	4.31	3.46	3.20	2.72	-0.18	0.09	0.55	1.52	1.64
HCOOH (Formic acid)	-0.59	2.28	1.53	1.06	0.69	-0.82	-0.90	-0.77	0.15	0.28
He (Helium atom)	-2.63	-1.24	-1.34	-1.23	-1.36	-2.94	-3.08	-2.80	-1.42	-1.26
HF (Hydrogen fluoride)	-0.64	1.26	0.96	0.51	0.71	-0.88	-0.98	-0.79	0.29	0.38
Li (Lithium atom)	0.62	2.17	1.35	1.03	1.52	-0.28	-0.27	-0.20	0.27	23.96
Mg (Magnesium atom)	-0.24	1.76	1.34	0.97	0.92	-0.39	-0.40	-0.30	0.34	0.35
N (Nitrogen atom)	-0.34	4.91	4.13	3.12	3.16	-0.17	0.00	0.47	1.69	3.19
N2 (Nitrogen diatomic)	-2.32	2.69	1.96	1.49	1.01	-2.05	-1.79	-1.29	-0.63	-0.81
N2H4 (Hydrazine)	-0.46	1.31	0.95	0.53	0.68	-0.75	-0.83	-0.67	0.36	0.45
N2O (Nitrous oxide)	-2.05	2.31	1.56	1.07	0.84	-1.64	-1.71	-1.37	-0.25	-0.17
Na (Sodium atom)	0.54	2.36	1.00	0.82	1.71	-0.25	-0.25	-0.21	0.21	18.24
NaCl (Sodium Chloride)	0.64	2.49	2.27	1.90	2.03	0.40	0.31	0.47	1.67	1.68
Ne (Neon atom)	-5.32	-2.06	-2.33	-3.70	-2.65	-5.78	-5.79	-5.55	-3.78	-3.99
NF3 (Nitrogen trifluoride)	-2.04	1.81	1.02	0.26	0.06	-2.18	-2.27	-2.01	-0.65	-0.55
NH (Imidogen)	0.14	5.39	4.32	3.50	3.31	0.09	0.34	0.80	1.80	1.80
NH2 (Amino radical)	0.54	5.75	4.54	3.54	3.45	0.32	0.60	1.07	1.95	1.17
NH3 (Ammonia)	-0.57	1.02	0.73	0.35	0.52	-0.83	-0.91	-0.76	0.20	0.33
NO (Nitric oxide)	-0.43	4.57	4.24	3.79	3.18	-0.06	0.25	0.83	1.45	-0.36
NO2 (Nitrogen dioxide)	1.47	5.95	5.06	4.59	4.35	1.40	1.66	2.11	3.01	1.82
O (Oxygen atom)	1.24	7.70	6.49	4.97	5.13	1.64	1.87	2.41	3.04	1.64
O2 (Oxygen diatomic)	-0.14	5.42	4.51	3.96	3.44	0.17	0.49	1.05	1.61	-0.30
O3 (Ozone)	2.30	6.98	6.21	6.01	5.62	2.67	2.94	3.40	4.11	2.34
OCS (Carbonyl sulfide)	-0.86	2.62	1.93	1.54	1.23	-1.26	-1.20	-0.81	0.02	0.11
OH (Hydroxyl radical)	1.60	7.79	6.46	5.14	5.04	1.67	1.93	2.47	2.94	1.22
P (Phosphorus atom)	0.61	4.59	3.74	3.41	3.25	0.65	0.92	1.25	2.54	4.19
P2 (Phosphorus diatomic)	0.46	4.01	3.42	3.23	2.79	0.46	0.63	0.96	1.74	0.68
PF3 (Phosphorus trifluoride)	-1.23	1.51	0.86	0.39	0.32	-1.52	-1.57	-1.36	-0.27	-0.20
PH3 (Phosphine)	-0.52	1.01	0.66	0.26	0.45	-0.79	-0.86	-0.72	0.17	0.34

S (Sulfur atom)	1.95	6.61	5.64	5.26	4.89	2.03	2.36	2.80	3.57	2.61
S2 (Sulfur diatomic)	1.45	5.28	4.51	4.33	3.86	1.32	1.55	1.94	2.81	1.57
Si (Silicon atom)	1.34	4.52	4.36	4.04	3.51	0.89	1.13	1.55	2.39	4.12
Si2H6 (Disilane)	-0.66	1.08	0.65	0.23	0.37	-0.84	-0.91	-0.78	0.14	0.35
SiF2 (Silicon difluoride)	0.07	3.64	3.01	2.73	2.40	-0.09	0.10	0.44	1.34	0.58
SiF4 (Silicon tetrafluoride)	-0.81	1.75	1.19	0.60	0.78	-1.16	-1.22	-1.02	0.27	0.27
SiH3 (Silyl)	0.82	4.41	3.54	3.38	3.01	1.07	1.19	1.30	2.85	6.34
SiH4 (Silane)	-0.59	0.78	0.46	0.14	0.29	-0.83	-0.91	-0.78	0.08	0.29
SiO (Silicon monoxide)	0.01	3.45	2.87	2.55	2.26	-0.14	0.03	0.35	1.24	0.58
SO2 (Sulfur dioxide)	0.87	5.13	4.42	4.18	3.76	0.95	1.20	1.64	2.44	1.09
MAE		3.15	2.53	2.87	1.96	0.29	0.34	0.42	1.26	1.80
MSE		3.15	2.53	2.87	1.95	-0.07	-0.03	0.24	1.25	1.75
RMS		3.44	2.81	8.90	2.15	0.37	0.41	0.56	1.80	5.57

Table S6. Fundamental gaps (1) [in eV] of the 121 molecules studied. The reference values are calculated by CCSD.

Molecule	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	5.55	5.44	5.49	5.55	5.56	5.69	5.67	5.62	5.47	5.50
AlCl3 (Aluminum trichloride)	12.23	10.70	10.57	11.47	11.08	12.48	12.20	11.84	11.79	11.83
Ar (Argon atom)	18.49	18.56	18.29	18.93	18.36	18.67	18.62	18.51	18.32	17.93
B (Boron atom)	8.02	7.96	8.05	8.34	8.27	8.27	8.27	8.21	8.06	7.96
BCl3 (Borane, trichloro-)	12.22	10.98	10.82	11.32	11.29	12.13	11.92	11.70	11.82	12.09
Be (Beryllium atom)	9.67	9.09	8.99	9.14	9.18	9.35	9.22	9.08	9.36	9.45
BF3 (Borane, trifluoro-)	17.38	15.43	15.04	15.33	15.84	16.69	16.53	16.34	16.88	17.70
C (Carbon atom)	10.02	9.92	9.95	10.09	10.17	10.16	10.16	10.13	10.05	10.06
C2F4 (Tetrafluoroethylene)	11.98	11.23	10.86	11.67	11.29	11.68	11.71	11.62	11.83	12.59
C2H2 (Acetylene)	13.33	12.34	11.79	11.64	11.79	11.91	11.94	11.92	11.99	13.50
C2H2O2 (Ethanedial)	10.23	8.96	8.94	9.22	9.41	9.91	9.82	9.66	9.87	10.35
C2H4 (Ethylene)	12.32	11.57	11.08	11.08	11.16	11.12	11.14	11.29	11.27	12.24
C2H4O (Ethylene oxide)	11.54	11.24	10.85	11.10	11.04	11.31	11.27	11.19	11.55	11.77
C2H4S (Thiirane)	9.80	9.74	9.37	9.63	9.51	9.67	9.67	9.62	9.84	9.91
C2H5N (Aziridine)	10.35	10.33	9.98	10.25	10.14	10.40	10.36	10.27	10.46	10.34
C2H6 (Ethane)	13.46	12.49	12.33	12.88	12.75	13.25	13.18	13.02	13.14	13.14
C2HF3 (Trifluoroethylene)	11.05	10.80	10.35	11.50	10.68	10.81	10.84	10.79	12.04	12.36
C2N2 (Cyanogen)	13.80	13.18	12.98	13.11	13.03	13.33	13.26	13.20	13.47	13.70
C3H4 (Cyclopropene)	11.66	10.52	10.15	11.18	10.27	10.43	10.43	10.36	10.49	11.79
C3H6 (Cyclopropane)	11.56	11.58	11.18	11.48	11.31	11.59	11.58	11.49	11.57	11.31
C3H8 (Propane)	12.83	11.61	11.47	12.00	11.99	12.63	12.53	12.33	12.42	12.52
C3O2 (Carbon suboxide)	11.35	11.70	11.51	11.61	11.43	11.69	11.72	11.70	11.77	11.49
C4H2 (Diacetylene)	11.47	10.83	10.57	10.86	10.70	10.68	10.67	10.99	11.18	11.45
C4H4O (Furan)	9.68	9.71	9.25	9.39	9.30	9.51	9.50	9.45	10.51	10.75
C4H6 (Cyclobutene)	11.86	10.18	9.80	10.22	9.88	10.07	10.08	10.03	10.67	11.97
C4N2 (2-Butynedinitrile)	11.47	10.55	10.42	10.57	10.57	10.94	10.87	10.78	11.05	11.33
CCl4 (Carbon tetrachloride)	12.29	10.42	10.31	10.87	10.93	12.35	12.07	11.66	11.88	12.64
CF2Cl2 (Difluorodichloromethane)	13.32	12.16	11.92	12.55	12.41	13.50	13.33	13.04	13.16	13.23
CF2O (Carbonic difluoride)	15.97	14.34	13.92	14.42	14.25	14.70	14.66	14.57	15.18	15.58
CF3Br (Bromotrifluoromethane)	12.83	12.42	12.10	12.29	12.42	12.81	12.76	12.64	12.69	12.99
CF3Cl (Methane, chlorotrifluoro-)	14.15	13.63	13.29	13.92	13.74	14.22	14.18	14.07	14.21	14.07
CF4 (Carbon tetrafluoride)	18.11	15.95	15.56	16.43	16.54	17.35	17.31	17.12	17.74	18.69
CFCl3 (Trichloromonofluoromethane)	12.64	11.06	10.90	11.56	11.44	12.75	12.50	12.14	12.34	12.95
CH2CCH2 (Allene)	10.72	10.86	10.45	10.66	10.53	10.70	10.71	10.67	11.07	10.60
CH2CCl2 (Ethene, 1,1-dichloro-)	10.97	10.51	9.90	10.60	10.13	10.55	10.49	10.37	10.48	10.42

CH2CF2 (Ethene, 1,1-difluoro-)	11.64	11.22	10.74	10.84	10.96	11.09	11.11	11.07	11.24	12.52
CH2CHCHO (Acrolein)	10.58	9.87	9.74	9.92	9.93	10.16	10.10	10.05	10.21	10.43
CH2CHCl (Ethene, chloro-)	10.97	11.11	10.22	11.11	10.36	10.66	10.62	10.53	11.37	11.57
CH2CHF (Ethene, fluoro-)	11.39	11.25	10.78	11.78	11.81	11.00	11.02	10.97	12.14	12.41
CH2Cl2 (Methylene chloride)	12.17	11.19	10.99	11.54	11.58	12.29	12.17	11.97	12.10	12.05
CH2CO (Ketene)	10.20	10.54	10.12	10.17	10.17	10.32	10.33	10.28	10.68	11.00
CH2F2 (Methane, difluoro-)	14.27	13.11	12.80	13.19	13.43	13.78	13.75	13.62	14.04	14.52
CH3 (Methyl radical)	9.95	9.73	9.96	10.08	9.91	9.94	9.90	9.87	9.85	9.66
CH3CCCH3 (2-Butyne)	10.32	9.92	9.60	9.77	10.34	10.09	10.08	10.01	10.20	10.56
CH3CCH (Propyne)	10.94	10.94	10.55	10.72	10.67	10.85	10.85	10.79	10.90	11.23
CH3CH2Cl (Ethyl chloride)	11.64	11.64	10.98	11.58	11.31	11.70	11.66	11.56	11.67	11.44
CH3CH2OH (Ethanol)	11.29	10.75	10.50	10.87	10.88	11.27	11.21	11.08	11.29	11.30
CH3Cl (Methyl chloride)	11.90	11.69	11.41	11.79	11.64	11.96	11.93	11.85	11.96	12.67
CH3COCl (Acetyl Chloride)	12.14	11.28	10.99	11.28	11.23	11.62	11.57	11.45	11.84	12.77
CH3F (Methyl fluoride)	14.04	13.41	13.10	13.39	13.51	13.80	13.76	13.66	13.92	14.11
CH3NHCH3 (Dimethylamine)	9.55	9.41	9.12	9.37	9.32	9.64	9.60	9.50	9.60	9.62
CH3NO2 (Methane, nitro-)	11.69	11.20	10.93	11.19	11.39	12.18	12.11	11.94	12.06	12.47
CH3OCH3 (Dimethyl ether)	10.69	10.39	10.09	10.38	10.36	10.70	10.66	10.56	10.69	10.63
CH3OH (Methyl alcohol)	11.57	11.35	11.02	11.21	11.28	11.57	11.53	11.43	11.62	11.68
CH3SH (Methanethiol)	9.90	9.86	9.56	9.97	9.72	9.99	9.99	9.94	9.97	9.75
CH3SiH3 (Methyl silane)	12.26	11.75	11.57	12.02	11.94	12.82	12.74	12.57	12.19	12.41
CH4 (Methane)	15.01	14.67	14.40	14.79	14.66	14.86	14.85	14.78	14.90	14.89
CHCl3 (Chloroform)	12.18	10.90	10.74	11.32	11.25	12.30	12.10	11.80	11.97	12.08
CHF3 (Methane, trifluoro-)	15.58	14.32	13.95	14.29	14.65	15.04	14.99	15.77	15.29	15.90
CHONH2 (Formamide)	10.67	10.82	10.40	11.59	10.52	10.71	10.67	10.58	12.01	12.26
Cl (Chlorine atom)	9.33	9.42	9.32	9.28	9.40	9.39	9.38	9.39	9.38	9.44
Cl2 (Chlorine diatomic)	11.00	10.41	10.30	10.73	10.52	10.96	10.87	10.79	10.94	11.03
ClF (Chlorine monofluoride)	12.47	11.96	11.79	12.20	12.06	12.29	12.28	12.27	12.54	12.73
ClF3 (Chlorine trifluoride)	12.05	11.05	10.93	11.28	11.37	11.70	11.69	11.63	12.01	12.47
ClO (Monochlorine monoxide)	8.99	8.88	8.80	8.92	8.97	9.00	9.01	9.01	8.97	9.08
CO (Carbon monoxide)	15.49	15.08	14.77	14.83	15.18	15.71	15.64	15.37	15.44	15.98
CO2 (Carbon dioxide)	14.61	14.73	14.31	14.89	14.47	14.90	14.84	14.75	14.89	15.02
CS (Carbon monosulfide)	11.43	11.37	11.19	11.22	11.33	12.67	12.59	11.39	11.43	11.65
CS2 (Carbon disulfide)	9.91	10.21	10.00	10.27	9.91	11.23	9.85	9.94	10.09	9.94
F (Fluorine atom)	14.08	13.89	14.00	14.13	14.20	14.02	14.07	14.13	14.22	14.16
F2 (Fluorine diatomic)	15.66	14.86	14.68	15.07	15.11	15.19	15.26	15.29	15.74	16.15
F2O (Difluorine monoxide)	13.93	12.93	12.77	13.20	13.32	13.56	13.59	13.58	14.08	14.63
FCN (Cyanogen fluoride)	14.21	14.12	13.73	14.22	13.87	14.17	14.16	14.10	14.27	14.37

H (Hydrogen atom)	12.86	12.19	12.90	13.12	12.76	13.00	12.91	12.87	12.96	12.89
H2CO (Formaldehyde)	11.43	11.44	11.24	11.50	11.30	11.84	11.42	11.66	11.82	12.08
H2CS (Thioformaldehyde)	9.05	9.00	8.83	8.98	8.86	8.84	8.87	8.91	9.04	9.21
H2O (Water)	13.21	13.69	13.18	13.24	13.20	13.41	13.35	13.27	13.37	13.41
H2O2 (Hydrogen peroxide)	12.71	12.05	11.70	12.06	12.21	12.47	12.43	12.32	12.77	13.21
H2S (Hydrogen sulfide)	10.88	11.07	10.73	11.12	10.81	11.03	11.03	10.99	11.02	10.83
HCCCN (Cyanoacetylene)	12.07	11.82	11.56	11.74	11.68	12.04	11.90	11.91	12.14	12.38
HCCF (Fluoroacetylene)	11.90	11.98	11.51	12.74	11.65	11.76	11.79	11.76	13.10	13.37
HCl (Hydrogen sulfide)	13.21	13.42	13.06	13.42	13.14	13.37	13.36	13.31	13.38	13.28
HCN (Hydrogen cyanide)	14.11	14.65	14.09	14.77	14.05	14.03	14.04	14.01	15.09	15.40
HCO (Formyl radical)	9.73	9.58	9.72	9.81	9.93	9.96	9.95	9.92	9.87	9.98
HCOOH (Formic acid)	11.85	11.92	11.44	12.27	11.63	11.88	11.84	11.74	12.83	13.27
He (Helium atom)	27.20	26.83	26.79	27.32	27.31	27.30	27.26	27.21	27.19	27.02
HF (Hydrogen fluoride)	16.76	17.35	16.76	16.71	16.78	16.94	16.85	16.77	16.86	16.87
Li (Lithium atom)	4.72	4.95	5.07	4.58	5.07	4.93	4.82	4.86	4.89	5.43
Mg (Magnesium atom)	7.77	7.85	7.63	7.73	7.80	7.96	7.89	7.69	8.03	7.98
N (Nitrogen atom)	14.81	14.65	14.45	14.89	14.43	14.60	14.65	14.69	14.67	14.34
N2 (Nitrogen diatomic)	18.03	17.30	17.03	17.24	17.29	17.79	17.77	17.62	17.77	18.89
N2H4 (Hydrazine)	10.30	9.88	9.65	10.15	9.94	10.29	10.24	10.12	10.33	10.46
N2O (Nitrous oxide)	14.82	14.32	13.87	14.74	13.92	14.25	14.23	14.18	14.83	14.72
Na (Sodium atom)	4.14	4.82	4.81	4.02	4.85	4.34	4.31	4.45	4.61	5.09
NaCl (Sodium Chloride)	8.48	8.92	8.52	8.83	8.51	8.61	8.63	8.60	8.67	8.37
Ne (Neon atom)	26.78	27.15	26.59	26.65	26.61	27.10	26.90	26.81	26.38	26.25
NF3 (Nitrogen trifluoride)	15.77	14.62	14.29	14.97	14.86	15.39	15.37	15.25	15.41	15.56
NH (Imidogen)	13.30	13.15	13.23	13.39	13.21	13.26	13.27	13.29	13.30	13.27
NH2 (Amino radical)	11.42	11.19	11.33	11.34	11.50	11.51	11.43	11.40	11.29	11.20
NH3 (Ammonia)	11.42	11.77	11.34	11.44	11.41	11.59	11.55	11.48	11.56	11.54
NO (Nitric oxide)	10.22	10.17	10.03	10.18	10.33	10.29	10.33	10.33	10.38	10.66
NO2 (Nitrogen dioxide)	10.10	9.88	9.97	10.22	10.26	10.25	10.27	10.30	10.34	10.55
O (Oxygen atom)	12.22	12.01	12.29	12.39	12.46	12.33	12.31	12.33	12.27	12.43
O2 (Oxygen diatomic)	12.75	12.67	12.66	13.07	12.97	12.95	12.99	13.03	13.13	13.14
O3 (Ozone)	10.99	10.85	10.70	10.69	10.70	10.74	10.73	10.74	10.90	11.26
OCS (Carbonyl sulfide)	12.07	12.53	12.24	12.53	12.01	12.26	12.26	12.23	12.59	12.49
OH (Hydroxyl radical)	11.36	11.21	11.33	11.41	11.49	11.41	11.41	11.42	11.43	11.30
P (Phosphorus atom)	9.83	9.53	9.61	9.96	9.43	9.67	9.58	9.54	9.46	9.20
P2 (Phosphorus diatomic)	9.98	10.16	9.93	10.01	9.82	9.63	10.19	10.20	9.90	9.83
PF3 (Phosphorus trifluoride)	12.97	12.48	12.09	12.45	12.51	12.92	12.90	12.79	12.80	13.01
PH3 (Phosphine)	11.05	11.10	10.83	11.27	10.97	11.13	11.15	11.12	11.07	10.69

S (Sulfur atom)	8.26	8.22	8.27	8.23	8.35	8.36	8.34	8.33	8.32	8.33
S2 (Sulfur diatomic)	8.07	8.00	8.10	8.30	8.15	8.32	8.24	8.19	8.16	8.05
Si (Silicon atom)	6.75	6.78	6.70	6.67	6.77	6.85	6.84	6.80	6.72	6.76
Si2H6 (Disilane)	11.22	10.85	10.58	11.18	10.83	11.16	11.15	11.08	11.10	11.03
SiF2 (Silicon difluoride)	11.03	10.81	10.52	10.75	10.79	10.97	10.93	10.85	10.86	10.84
SiF4 (Silicon tetrafluoride)	17.72	15.23	14.91	15.88	15.87	16.98	16.85	16.56	17.18	18.25
SiH3 (Silyl)	8.02	7.80	8.01	8.13	7.99	7.98	7.97	7.96	8.08	7.96
SiH4 (Silane)	13.45	12.69	12.52	13.23	12.90	13.41	13.33	13.18	13.17	13.12
SiO (Silicon monoxide)	11.50	11.35	11.07	11.25	11.25	11.52	11.48	11.40	11.51	11.72
SO2 (Sulfur dioxide)	11.71	11.50	11.31	11.43	11.42	11.54	11.53	11.52	11.67	11.85
MAE		0.51	0.65	0.44	0.45	0.28	0.26	0.30	0.27	0.33
MSE		-0.39	-0.63	-0.29	-0.39	-0.09	-0.14	-0.22	-0.02	0.18
RMS		0.71	0.88	0.62	0.62	0.42	0.41	0.44	0.40	0.46

Table S7. Fundamental gaps (2) [in eV] of the 121 molecules studied. The reference values are calculated by CCSD.

Molecule	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	5.55	4.29	4.35	4.61	4.55	5.28	5.21	5.02	4.75	5.06
AlCl3 (Aluminum trichloride)	12.23	9.55	9.41	10.19	10.20	12.34	11.91	11.36	11.39	12.25
Ar (Argon atom)	18.49	15.04	14.88	15.48	15.98	17.79	17.37	16.64	16.95	18.30
B (Boron atom)	8.02	5.89	5.95	6.20	6.48	7.34	7.22	6.93	6.83	7.05
BCl3 (Borane, trichloro-)	12.22	10.42	9.79	10.18	10.87	11.68	11.50	11.33	11.68	12.28
Be (Beryllium atom)	9.67	7.06	6.92	7.06	7.46	9.18	8.94	8.57	8.16	9.14
BF3 (Borane, trifluoro-)	17.38	12.44	12.10	12.18	13.78	16.06	15.72	15.12	15.97	18.84
C (Carbon atom)	10.02	7.95	7.98	8.37	8.48	9.00	8.91	8.72	8.85	9.31
C2F4 (Tetrafluoroethylene)	11.98	8.74	8.09	9.09	9.53	11.66	11.40	10.80	10.86	13.36
C2H2 (Acetylene)	13.33	8.79	8.45	8.61	9.35	11.86	11.56	10.95	10.85	13.81
C2H2O2 (Ethanedial)	10.23	8.64	8.58	8.89	9.14	9.56	9.50	9.37	9.74	10.52
C2H4 (Ethylene)	12.32	8.52	8.19	8.29	8.98	11.25	10.95	10.56	10.37	12.73
C2H4O (Ethylene oxide)	11.54	7.98	7.70	8.03	9.01	11.32	11.05	10.45	10.97	13.57
C2H4S (Thiirane)	9.80	7.09	6.80	7.07	7.68	9.90	9.58	9.01	9.00	10.82
C2H5N (Aziridine)	10.35	7.46	7.21	7.52	8.28	10.52	10.21	9.62	9.75	11.41
C2H6 (Ethane)	13.46	9.75	9.61	10.10	10.77	13.10	12.80	12.20	12.17	13.77
C2HF3 (Trifluoroethylene)	11.05	8.04	7.68	9.15	8.73	10.79	10.55	9.99	11.28	13.03
C2N2 (Cyanogen)	13.80	12.67	12.49	12.75	12.68	13.16	13.05	12.93	13.17	13.48
C3H4 (Cyclopropene)	11.66	7.76	7.49	9.05	8.29	10.54	10.26	9.71	9.68	12.07
C3H6 (Cyclopropane)	11.56	8.79	8.49	8.80	9.45	11.82	11.53	10.94	10.76	12.12
C3H8 (Propane)	12.83	9.23	9.10	9.54	10.25	12.60	12.31	11.72	11.64	13.06
C3O2 (Carbon suboxide)	11.35	11.40	11.13	11.48	11.25	11.74	11.51	11.04	10.98	11.38
C4H2 (Diacetylene)	11.47	9.45	9.08	9.28	9.69	10.84	10.59	10.64	10.71	11.62
C4H4O (Furan)	9.68	7.29	6.93	7.15	7.66	9.80	9.54	9.04	9.96	11.35
C4H6 (Cyclobutene)	11.86	7.66	7.37	7.81	8.16	10.40	10.13	9.59	9.94	12.34
C4N2 (2-Butynedinitrile)	11.47	10.30	10.18	10.36	10.39	10.87	10.77	10.64	10.88	11.27
CCl4 (Carbon tetrachloride)	12.29	9.79	9.57	10.45	10.36	12.06	11.79	11.35	11.57	12.84
CF2Cl2 (Difluorodichloromethane)	13.32	10.37	10.09	10.58	11.08	13.41	13.02	12.37	12.45	14.01
CF2O (Carbonic difluoride)	15.97	11.11	10.79	11.36	12.19	14.35	14.05	13.42	14.48	17.12
CF3Br (Bromotrifluoromethane)	12.83	10.36	10.00	10.56	10.99	12.74	12.43	11.92	12.22	13.16
CF3Cl (Methane, chlorotrifluoro-)	14.15	10.97	10.69	11.36	11.80	14.07	13.70	13.09	13.30	14.94
CF4 (Carbon tetrafluoride)	18.11	13.14	12.79	13.55	14.56	16.84	16.63	16.02	16.91	19.89
CFCl3 (Trichloromonofluoromethane)	12.64	9.97	9.74	10.42	10.60	12.50	12.21	11.74	11.93	13.13
CH2CCH2 (Allene)	10.72	8.18	7.89	8.32	8.73	11.00	10.72	10.17	10.38	11.35
CH2CCl2 (Ethene, 1,1-dichloro-)	10.97	9.29	7.87	9.29	8.66	10.76	10.48	9.95	9.90	11.19

CH2CF2 (Ethene, 1,1-difluoro-)	11.64	8.34	7.99	8.18	8.96	11.12	10.85	10.29	10.35	13.17
CH2CHCHO (Acrolein)	10.58	8.82	8.67	9.19	9.48	10.21	10.12	9.93	10.46	11.33
CH2CHCl (Ethene, chloro-)	10.97	9.53	7.86	9.43	8.67	10.76	10.48	9.94	10.90	11.85
CH2CHF (Ethene, fluoro-)	11.39	8.32	7.97	9.62	10.24	11.04	10.76	10.20	11.53	12.84
CH2Cl2 (Methylene chloride)	12.17	9.21	8.98	9.38	9.96	12.13	11.80	11.18	11.26	12.85
CH2CO (Ketene)	10.20	8.02	7.61	7.80	8.20	10.29	10.03	9.49	9.75	11.37
CH2F2 (Methane, difluoro-)	14.27	9.91	9.65	10.10	11.14	13.33	13.07	12.46	13.00	15.33
CH3 (Methyl radical)	9.95	7.72	7.80	7.84	8.24	8.96	8.81	8.56	8.74	8.91
CH3CCCH3 (2-Butyne)	10.32	7.42	7.17	7.32	8.51	10.38	10.11	9.55	9.43	10.94
CH3CCH (Propyne)	10.94	8.14	7.81	8.23	8.61	10.98	10.67	10.09	9.91	11.62
CH3CH2Cl (Ethyl chloride)	11.64	8.62	8.40	8.90	9.42	11.71	11.38	10.77	10.80	12.28
CH3CH2OH (Ethanol)	11.29	7.80	7.55	7.89	8.86	11.18	10.90	10.27	10.59	12.58
CH3Cl (Methyl chloride)	11.90	8.84	8.62	8.81	9.62	11.85	11.51	10.90	10.97	13.43
CH3COCl (Acetyl Chloride)	12.14	9.20	8.82	9.20	9.61	11.73	11.47	10.90	11.48	12.53
CH3F (Methyl fluoride)	14.04	9.84	9.58	9.90	11.04	13.28	13.02	12.41	12.90	15.07
CH3NHCH3 (Dimethylamine)	9.55	6.62	6.40	6.73	7.50	9.82	9.53	8.93	8.97	10.34
CH3NO2 (Methane, nitro-)	11.69	9.04	8.62	8.96	10.03	11.92	11.66	11.04	11.77	11.47
CH3OCH3 (Dimethyl ether)	10.69	7.44	7.19	7.54	8.45	10.77	10.51	9.92	10.15	12.06
CH3OH (Methyl alcohol)	11.57	7.98	7.72	7.96	9.05	11.32	11.04	10.41	10.78	12.92
CH3SH (Methanethiol)	9.90	7.21	7.00	7.30	7.88	10.09	9.77	9.19	9.03	10.41
CH3SiH3 (Methyl silane)	12.26	9.49	9.17	9.48	10.15	12.53	12.24	11.65	11.38	12.72
CH4 (Methane)	15.01	11.12	10.95	11.52	12.15	14.53	14.20	13.56	13.61	15.42
CHCl3 (Chloroform)	12.18	9.51	9.29	9.71	10.19	12.18	11.82	11.22	11.42	12.92
CHF3 (Methane, trifluoro-)	15.58	11.25	10.93	11.30	12.44	14.59	14.33	13.72	14.24	16.71
CHONH2 (Formamide)	10.67	7.71	7.43	8.93	8.66	10.73	10.45	9.84	11.64	13.53
Cl (Chlorine atom)	9.33	8.46	8.38	8.33	8.56	8.73	8.69	8.63	8.71	9.14
Cl2 (Chlorine diatomic)	11.00	9.42	9.29	9.84	9.83	10.65	10.53	10.34	10.50	11.08
ClF (Chlorine monofluoride)	12.47	10.62	10.48	11.05	11.13	11.89	11.78	11.60	11.92	12.70
ClF3 (Chlorine trifluoride)	12.05	10.57	10.39	10.88	11.02	11.41	11.39	11.32	11.73	12.36
ClO (Monochlorine monoxide)	8.99	6.69	8.10	8.15	8.35	8.50	8.48	8.44	8.46	8.84
CO (Carbon monoxide)	15.49	12.06	11.78	12.04	13.02	15.18	14.83	14.17	14.46	16.52
CO2 (Carbon dioxide)	14.61	11.56	11.24	11.81	12.39	14.40	14.11	13.53	13.84	15.78
CS (Carbon monosulfide)	11.43	10.33	10.21	10.62	10.80	12.82	12.50	11.21	11.37	12.01
CS2 (Carbon disulfide)	9.91	9.42	9.23	9.84	9.41	11.39	9.67	9.65	9.74	9.56
F (Fluorine atom)	14.08	11.76	11.83	12.00	12.32	12.29	12.32	12.33	12.79	13.46
F2 (Fluorine diatomic)	15.66	13.19	12.96	13.40	14.01	14.44	14.43	14.34	14.87	15.56
F2O (Difluorine monoxide)	13.93	11.50	11.25	11.98	12.44	13.13	13.09	12.94	13.66	14.87
FCN (Cyanogen fluoride)	14.21	11.17	10.88	11.18	11.84	13.79	13.45	12.85	13.11	14.72

H (Hydrogen atom)	12.86	9.03	9.30	9.28	9.78	10.51	10.31	10.07	10.44	10.81
H2CO (Formaldehyde)	11.43	9.18	8.91	9.21	9.04	11.53	10.86	10.91	11.35	12.88
H2CS (Thioformaldehyde)	9.05	8.17	8.05	8.40	8.32	8.75	8.66	8.56	8.74	9.31
H2O (Water)	13.21	9.29	9.00	9.28	10.40	12.63	12.29	11.61	12.25	14.84
H2O2 (Hydrogen peroxide)	12.71	8.45	8.17	8.49	9.68	11.94	11.63	10.96	11.68	14.65
H2S (Hydrogen sulfide)	10.88	8.04	7.82	8.17	8.69	10.90	10.56	9.96	9.82	11.29
HCCCN (Cyanoacetylene)	12.07	10.59	10.20	10.38	10.84	11.96	11.66	11.58	11.76	12.40
HCCF (Fluoroacetylene)	11.90	8.75	8.41	10.00	9.39	11.65	11.36	10.77	12.09	13.79
HCl (Hydrogen sulfide)	13.21	9.95	9.72	10.12	10.72	12.96	12.58	11.94	12.14	13.89
HCN (Hydrogen cyanide)	14.11	10.93	10.61	11.89	11.55	13.70	13.35	12.73	13.99	15.81
HCO (Formyl radical)	9.73	7.80	7.76	7.83	8.50	9.08	8.97	8.76	9.00	9.72
HCOOH (Formic acid)	11.85	8.51	8.16	9.56	9.47	11.74	11.46	10.85	12.33	14.56
He (Helium atom)	27.20	19.95	19.95	20.87	21.92	23.76	23.47	22.80	24.26	27.17
HF (Hydrogen fluoride)	16.76	11.95	11.65	12.01	13.33	15.37	15.08	14.42	15.57	18.62
Li (Lithium atom)	4.72	4.09	4.08	4.16	4.22	4.66	4.59	4.51	4.27	4.73
Mg (Magnesium atom)	7.77	5.87	5.62	5.65	6.10	7.67	7.59	7.29	6.89	7.79
N (Nitrogen atom)	14.81	11.52	11.39	11.74	12.08	12.75	12.69	12.54	13.19	14.25
N2 (Nitrogen diatomic)	18.03	14.64	14.25	14.36	14.42	16.99	16.68	15.96	16.25	18.73
N2H4 (Hydrazine)	10.30	7.04	6.87	7.29	8.01	10.15	9.83	9.21	9.49	11.37
N2O (Nitrous oxide)	14.82	11.15	10.79	12.50	11.83	13.81	13.54	12.99	14.12	14.65
Na (Sodium atom)	4.14	3.99	3.87	3.78	4.04	4.14	4.24	4.23	4.28	4.75
NaCl (Sodium Chloride)	8.48	6.32	6.07	6.14	6.83	8.57	8.25	7.69	7.92	9.24
Ne (Neon atom)	26.78	21.35	21.04	21.55	22.93	24.07	23.90	23.45	24.94	27.87
NF3 (Nitrogen trifluoride)	15.77	11.69	11.41	11.94	12.79	14.96	14.66	14.03	14.41	16.87
NH (Imidogen)	13.30	10.68	10.71	10.97	11.31	11.79	11.71	11.58	12.05	12.67
NH2 (Amino radical)	11.42	9.59	9.69	9.81	10.14	10.50	10.39	10.25	10.55	11.09
NH3 (Ammonia)	11.42	8.02	7.79	8.20	8.96	11.24	10.90	10.24	10.50	12.54
NO (Nitric oxide)	10.22	4.95	8.23	8.35	9.03	9.43	9.40	9.26	9.59	10.41
NO2 (Nitrogen dioxide)	10.10	8.63	8.65	9.04	9.30	9.56	9.53	9.47	9.75	10.39
O (Oxygen atom)	12.22	9.91	10.07	10.38	10.59	10.75	10.69	10.63	10.96	11.29
O2 (Oxygen diatomic)	12.75	11.02	10.98	11.56	11.69	11.92	11.92	11.89	12.34	12.78
O3 (Ozone)	10.99	10.30	10.16	10.25	10.26	10.32	10.32	10.32	10.22	9.51
OCS (Carbonyl sulfide)	12.07	10.88	10.51	10.83	10.27	12.16	11.88	11.39	12.02	12.16
OH (Hydroxyl radical)	11.36	9.44	9.52	9.61	9.96	10.10	10.05	9.99	10.34	10.96
P (Phosphorus atom)	9.83	8.04	8.07	8.41	8.23	9.06	8.84	8.59	8.66	8.86
P2 (Phosphorus diatomic)	9.98	9.36	9.19	9.50	9.28	9.60	9.58	9.53	9.58	9.51
PF3 (Phosphorus trifluoride)	12.97	9.85	9.51	9.83	10.56	12.75	12.45	11.84	11.84	13.51
PH3 (Phosphine)	11.05	8.33	8.15	8.58	8.98	11.10	10.82	10.28	10.06	11.30

S (Sulfur atom)	8.26	7.24	7.27	7.36	7.48	7.75	7.67	7.58	7.64	7.84
S2 (Sulfur diatomic)	8.07	7.37	7.44	7.64	7.61	7.97	7.87	7.75	7.79	7.96
Si (Silicon atom)	6.75	4.79	5.73	5.86	5.91	6.41	6.33	6.18	6.07	6.34
Si2H6 (Disilane)	11.22	8.62	8.38	9.05	9.21	11.46	11.21	10.69	10.34	11.92
SiF2 (Silicon difluoride)	11.03	9.30	9.06	9.27	9.68	10.61	10.52	10.28	10.37	11.10
SiF4 (Silicon tetrafluoride)	17.72	12.96	12.66	13.42	14.27	16.57	16.30	15.68	16.33	19.08
SiH3 (Silyl)	8.02	6.73	6.82	7.06	7.03	7.59	7.48	7.30	7.30	7.50
SiH4 (Silane)	13.45	10.05	9.89	10.64	10.93	13.30	12.98	12.39	12.24	13.78
SiO (Silicon monoxide)	11.50	9.60	9.36	9.55	10.13	11.31	11.17	10.87	11.06	12.29
SO2 (Sulfur dioxide)	11.71	10.84	10.61	10.91	11.01	11.25	11.24	11.20	11.46	11.90
MAE		6.14	2.88	2.43	2.03	0.58	0.73	1.13	0.86	0.75
MSE		-5.46	-2.88	-2.43	-2.03	-0.47	-0.71	-1.13	-0.82	0.49
RMS		8.08	3.14	2.70	2.22	0.82	0.94	1.30	1.01	0.95

Table S8. Fundamental gaps (3) [in eV] of the 121 molecules studied. The reference values are calculated by CCSD.

Molecule	CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	5.55	0.10	0.33	0.77	1.52	5.92	5.67	5.10	3.04	1.85
AlCl3 (Aluminum trichloride)	12.23	5.71	5.80	6.71	7.43	12.57	12.18	11.43	9.74	12.07
Ar (Argon atom)	18.49	11.20	10.94	12.37	12.59	18.11	17.86	17.00	15.26	17.63
B (Boron atom)	8.02	0.18	0.55	1.61	2.48	8.04	7.60	6.67	4.74	3.66
BCl3 (Borane, trichloro-)	12.22	4.88	5.00	5.58	6.87	12.60	12.04	11.07	9.57	12.42
Be (Beryllium atom)	9.67	3.52	3.59	4.00	4.89	9.28	9.09	8.53	6.72	8.39
BF3 (Borane, trifluoro-)	17.38	9.59	9.27	9.98	11.43	16.16	16.07	15.31	14.37	17.95
C (Carbon atom)	10.02	0.07	0.52	1.44	3.05	9.37	8.75	7.59	6.13	7.69
C2F4 (Tetrafluoroethylene)	11.98	5.88	5.71	6.20	7.29	11.83	11.72	11.03	9.27	11.76
C2H2 (Acetylene)	13.33	6.80	6.79	7.32	8.14	12.05	11.83	11.20	9.78	11.63
C2H2O2 (Ethanedial)	10.23	1.80	1.94	2.48	4.18	9.93	9.45	8.45	7.34	11.41
C2H4 (Ethylene)	12.32	5.61	5.62	6.05	7.26	11.45	11.26	10.61	9.11	10.85
C2H4O (Ethylene oxide)	11.54	6.22	5.88	6.29	7.47	11.52	11.37	10.69	9.64	12.36
C2H4S (Thiirane)	9.80	4.39	4.41	4.85	6.00	10.13	9.93	9.27	7.70	9.66
C2H5N (Aziridine)	10.35	5.47	5.23	5.69	6.65	10.74	10.56	9.88	8.51	10.72
C2H6 (Ethane)	13.46	7.94	7.75	8.30	9.20	13.31	13.11	12.41	10.96	13.10
C2HF3 (Trifluoroethylene)	11.05	5.39	5.43	5.92	7.03	11.00	10.87	10.23	8.83	11.02
C2N2 (Cyanogen)	13.80	5.83	5.85	6.34	7.66	13.33	12.81	11.84	10.56	14.03
C3H4 (Cyclopropene)	11.66	4.92	5.00	5.53	6.70	10.75	10.58	9.95	8.52	10.33
C3H6 (Cyclopropane)	11.56	7.09	6.74	7.10	7.98	12.02	11.83	11.15	9.59	11.48
C3H8 (Propane)	12.83	7.44	7.29	7.85	8.74	12.80	12.61	11.93	10.46	12.49
C3O2 (Carbon suboxide)	11.35	4.67	4.71	5.13	6.33	11.48	11.07	10.27	8.87	11.52
C4H2 (Diacetylene)	11.47	4.78	4.80	5.24	6.37	10.98	10.81	10.26	8.81	10.58
C4H4O (Furan)	9.68	4.79	4.79	5.13	6.29	10.01	9.87	9.28	7.75	9.41
C4H6 (Cyclobutene)	11.86	5.34	5.38	5.82	6.73	10.61	10.44	9.81	8.31	10.08
C4N2 (2-Butynedinitrile)	11.47	4.45	4.47	4.88	6.07	11.31	10.85	9.99	8.64	11.85
CCl4 (Carbon tetrachloride)	12.29	4.94	4.96	5.39	6.90	12.68	12.16	11.16	9.81	12.57
CF2Cl2 (Difluorodichloromethane)	13.32	6.10	6.15	6.68	8.10	13.64	13.28	12.35	10.88	13.18
CF2O (Carbonic difluoride)	15.97	6.63	6.74	7.50	9.21	14.57	14.41	13.63	12.32	15.36
CF3Br (Bromotrifluoromethane)	12.83	5.77	5.81	6.48	7.60	13.05	12.70	11.83	10.27	12.74
CF3Cl (Methane, chlorotrifluoro-)	14.15	7.23	7.27	7.92	9.27	14.41	14.15	13.33	11.75	14.06
CF4 (Carbon tetrafluoride)	18.11	10.68	10.21	10.81	12.38	17.11	17.05	16.26	15.27	18.85
CFCl3 (Trichloromonofluoromethane)	12.64	5.25	5.29	5.76	7.23	12.97	12.47	11.49	10.11	12.73
CH2CCH2 (Allene)	10.72	5.70	5.70	6.13	7.25	11.20	11.02	10.38	8.87	10.71
CH2CCl2 (Ethene, 1,1-dichloro-)	10.97	4.71	4.75	5.17	6.37	11.02	10.85	10.23	8.66	10.44

CH2CF2 (Ethene, 1,1-difluoro-)	11.64	5.78	5.80	6.32	7.34	11.34	11.18	10.53	9.10	11.15
CH2CHCHO (Acrolein)	10.58	2.83	2.93	3.47	5.13	10.77	10.31	9.35	8.25	11.33
CH2CHCl (Ethene, chloro-)	10.97	4.93	4.97	5.41	6.63	11.01	10.84	10.21	8.69	10.45
CH2CHF (Ethene, fluoro-)	11.39	5.47	5.49	5.94	7.22	11.26	11.09	10.45	9.01	10.90
CH2Cl2 (Methylene chloride)	12.17	5.91	5.94	6.47	7.77	12.39	12.17	11.45	9.91	12.02
CH2CO (Ketene)	10.20	3.72	3.76	4.27	5.65	10.49	10.34	9.72	8.22	10.14
CH2F2 (Methane, difluoro-)	14.27	8.06	7.73	8.13	9.49	13.53	13.39	12.70	11.66	14.46
CH3 (Methyl radical)	9.95	1.76	2.48	3.29	4.28	10.00	9.51	8.58	6.61	6.44
CH3CCCH3 (2-Butyne)	10.32	5.70	5.40	5.80	6.56	10.57	10.39	9.74	8.23	10.08
CH3CCH (Propyne)	10.94	6.33	5.99	6.37	7.15	11.21	11.01	10.35	8.85	10.74
CH3CH2Cl (Ethyl chloride)	11.64	6.39	6.29	6.82	7.72	11.95	11.73	11.03	9.54	11.60
CH3CH2OH (Ethanol)	11.29	5.75	5.49	6.02	7.18	11.40	11.23	10.52	9.34	11.93
CH3Cl (Methyl chloride)	11.90	6.33	6.23	6.79	7.75	12.08	11.86	11.15	9.67	11.77
CH3COCl (Acetyl Chloride)	12.14	4.72	4.79	5.41	6.90	11.98	11.82	11.13	9.84	12.08
CH3F (Methyl fluoride)	14.04	8.01	7.67	8.14	9.40	13.48	13.34	12.64	11.60	14.23
CH3NHCH3 (Dimethylamine)	9.55	4.72	4.51	5.02	5.94	10.02	9.83	9.15	7.79	9.96
CH3NO2 (Methane, nitro-)	11.69	3.67	3.74	4.24	6.07	11.95	11.49	10.46	9.68	12.40
CH3OCH3 (Dimethyl ether)	10.69	5.60	5.34	5.82	6.90	10.97	10.82	10.14	8.96	11.41
CH3OH (Methyl alcohol)	11.57	5.85	5.59	6.12	7.29	11.52	11.35	10.64	9.49	12.12
CH3SH (Methanethiol)	9.90	4.86	4.72	5.26	6.05	10.31	10.10	9.42	7.78	9.63
CH3SiH3 (Methyl silane)	12.26	7.41	7.25	7.84	8.61	12.71	12.50	11.85	10.23	12.04
CH4 (Methane)	15.01	9.35	9.08	9.61	10.54	14.75	14.52	13.78	12.39	14.63
CHCl3 (Chloroform)	12.18	5.36	5.39	5.90	7.28	12.49	12.22	11.44	9.93	12.09
CHF3 (Methane, trifluoro-)	15.58	9.32	8.94	9.30	10.73	14.79	14.65	13.95	12.95	15.86
CHONH2 (Formamide)	10.67	5.13	5.19	5.67	6.80	10.98	10.82	10.12	9.00	11.27
Cl (Chlorine atom)	9.33	0.38	0.40	0.86	2.58	8.80	8.13	7.00	5.85	10.10
Cl2 (Chlorine diatomic)	11.00	3.00	3.08	3.51	5.05	10.88	10.33	9.32	8.07	11.76
ClF (Chlorine monofluoride)	12.47	3.31	3.42	4.03	5.74	11.80	11.27	10.21	9.18	13.19
ClF3 (Chlorine trifluoride)	12.05	3.05	3.14	3.65	5.51	11.51	11.03	9.98	9.18	13.79
ClO (Monochlorine monoxide)	8.99	0.35	0.33	0.75	2.78	8.72	8.23	7.15	5.98	10.63
CO (Carbon monoxide)	15.49	6.88	7.03	7.68	9.40	15.30	14.87	13.82	12.49	15.46
CO2 (Carbon dioxide)	14.61	8.49	8.19	8.90	9.87	14.59	14.42	13.69	12.21	14.82
CS (Carbon monosulfide)	11.43	3.86	3.99	4.40	6.06	11.90	11.38	10.37	8.86	12.64
CS2 (Carbon disulfide)	9.91	3.96	3.98	4.38	5.39	10.31	9.92	9.20	7.62	10.20
F (Fluorine atom)	14.08	0.09	1.01	2.80	4.74	11.32	10.93	9.73	10.11	16.44
F2 (Fluorine diatomic)	15.66	3.45	3.65	4.69	7.00	13.29	12.91	11.79	11.98	17.89
F2O (Difluorine monoxide)	13.93	3.24	3.42	4.27	6.51	12.80	12.36	11.23	11.05	16.55
FCN (Cyanogen fluoride)	14.21	7.37	7.20	8.03	8.92	14.03	13.78	12.97	11.35	13.83

H (Hydrogen atom)	12.86	5.26	6.90	-87.14	8.74	10.31	10.14	9.61	-5.00	-40.36
H2CO (Formaldehyde)	11.43	3.42	3.58	4.23	5.90	11.33	11.20	10.24	9.11	11.96
H2CS (Thioformaldehyde)	9.05	1.81	1.91	2.23	3.68	9.21	8.73	7.82	6.29	9.71
H2O (Water)	13.21	6.64	6.33	6.94	8.15	12.82	12.62	11.82	10.71	13.70
H2O2 (Hydrogen peroxide)	12.71	4.68	4.77	5.66	7.37	12.12	11.95	11.17	10.07	13.22
H2S (Hydrogen sulfide)	10.88	5.67	5.47	6.09	6.75	11.10	10.86	10.18	8.54	10.36
HCCCN (Cyanoacetylene)	12.07	5.17	5.19	5.65	6.87	12.19	11.82	10.93	9.51	11.86
HCCF (Fluoroacetylene)	11.90	6.56	6.28	6.79	7.69	11.85	11.66	10.99	9.59	11.67
HCl (Hydrogen sulfide)	13.21	7.10	6.94	7.64	8.50	13.15	12.88	12.13	10.64	12.82
HCN (Hydrogen cyanide)	14.11	7.88	7.89	8.48	9.75	13.91	13.69	12.98	11.66	13.72
HCO (Formyl radical)	9.73	1.27	1.70	2.03	3.80	9.56	9.06	8.06	6.53	8.99
HCOOH (Formic acid)	11.85	5.11	5.20	5.79	7.47	11.95	11.79	11.09	10.00	12.80
He (Helium atom)	27.20	17.27	17.10	17.77	19.36	24.07	23.99	23.08	22.03	25.41
HF (Hydrogen fluoride)	16.76	9.06	8.70	9.39	10.84	15.56	15.42	14.61	13.83	17.39
Li (Lithium atom)	4.72	1.41	1.88	2.19	2.13	5.62	5.58	5.41	3.90	-18.76
Mg (Magnesium atom)	7.77	3.44	3.36	3.75	4.37	7.75	7.72	7.38	5.85	7.05
N (Nitrogen atom)	14.81	3.94	4.17	5.48	6.61	13.10	12.70	11.63	10.07	11.22
N2 (Nitrogen diatomic)	18.03	8.21	8.31	8.86	10.95	17.18	16.66	15.54	14.58	17.98
N2H4 (Hydrazine)	10.30	4.52	4.35	4.96	5.94	10.39	10.19	9.44	8.02	10.54
N2O (Nitrous oxide)	14.82	6.81	6.83	7.40	8.79	14.04	13.90	13.06	11.54	13.94
Na (Sodium atom)	4.14	1.13	2.04	2.14	1.78	5.08	5.17	5.10	3.98	-13.04
NaCl (Sodium Chloride)	8.48	3.38	3.01	3.36	4.28	8.80	8.60	7.90	6.12	8.31
Ne (Neon atom)	26.78	16.13	15.68	17.44	18.30	24.42	24.29	23.47	22.46	26.82
NF3 (Nitrogen trifluoride)	15.77	7.29	7.41	8.31	10.02	15.25	15.10	14.25	12.77	15.83
NH (Imidogen)	13.30	3.02	3.60	4.63	6.06	12.38	11.88	10.81	9.48	12.17
NH2 (Amino radical)	11.42	1.96	2.68	3.78	5.11	11.31	10.73	9.65	8.34	11.79
NH3 (Ammonia)	11.42	5.73	5.46	6.02	6.99	11.45	11.22	10.46	9.13	11.57
NO (Nitric oxide)	10.22	0.38	0.28	0.71	3.00	9.18	8.64	7.48	6.59	11.75
NO2 (Nitrogen dioxide)	10.10	1.09	1.43	1.87	3.82	9.71	9.24	8.20	7.11	11.73
O (Oxygen atom)	12.22	0.28	1.11	2.79	4.14	10.71	10.20	9.01	8.18	12.47
O2 (Oxygen diatomic)	12.75	1.98	2.31	3.11	5.28	11.56	11.04	9.88	9.39	14.83
O3 (Ozone)	10.99	1.72	1.79	2.06	4.08	10.05	9.55	8.49	7.55	11.41
OCS (Carbonyl sulfide)	12.07	5.52	5.57	6.11	7.24	12.49	12.19	11.34	9.82	11.63
OH (Hydroxyl radical)	11.36	0.14	0.93	2.30	3.98	10.46	9.92	8.74	8.17	13.19
P (Phosphorus atom)	9.83	2.15	2.56	3.02	3.87	9.42	8.87	8.01	5.82	5.88
P2 (Phosphorus diatomic)	9.98	3.71	3.72	3.99	5.06	10.04	9.67	8.94	7.26	9.86
PF3 (Phosphorus trifluoride)	12.97	6.47	6.48	7.06	8.24	12.93	12.75	12.00	10.32	12.55
PH3 (Phosphine)	11.05	6.22	6.05	6.61	7.22	11.30	11.12	10.49	8.79	10.41

S (Sulfur atom)	8.26	0.05	0.52	0.87	2.32	8.06	7.48	6.53	4.96	7.99
S2 (Sulfur diatomic)	8.07	1.01	1.31	1.56	2.95	8.41	7.88	6.96	5.32	8.64
Si (Silicon atom)	6.75	0.27	0.24	0.53	1.77	7.05	6.60	5.76	3.86	3.70
Si2H6 (Disilane)	11.22	6.64	6.53	7.11	7.72	11.65	11.49	10.89	9.14	10.77
SiF2 (Silicon difluoride)	11.03	4.09	4.11	4.49	5.74	10.95	10.57	9.76	8.09	10.74
SiF4 (Silicon tetrafluoride)	17.72	9.69	9.49	10.35	11.74	16.73	16.58	15.80	14.78	18.32
SiH3 (Silyl)	8.02	1.35	1.84	2.05	3.14	7.73	7.41	6.86	4.40	2.59
SiH4 (Silane)	13.45	8.22	8.06	8.72	9.39	13.49	13.28	12.60	11.02	12.83
SiO (Silicon monoxide)	11.50	4.62	4.60	5.02	6.34	11.56	11.20	10.39	8.85	11.76
SO2 (Sulfur dioxide)	11.71	3.58	3.61	3.90	5.62	11.34	10.87	9.89	8.69	12.83
MAE		7.07	7.03	7.22	5.19	0.51	0.64	1.39	2.82	1.57
MSE		-7.07	-7.03	-7.22	-5.19	-0.27	-0.56	-1.36	-2.82	-0.92
RMS		7.32	7.25	11.25	5.35	0.77	0.93	1.61	3.21	5.66

Table S9. Optical gaps [in eV] of the 121 molecules studied. The reference values are calculated by EOM-CCSD.

Molecule	EOM-CCSD	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	3.16	2.78	2.73	3.16	2.77	3.27	3.22	2.99	2.67	2.28
AlCl3 (Aluminum trichloride)	8.13	6.46	6.52	7.35	7.03	8.12	7.89	7.64	7.43	7.31
Ar (Argon atom)	12.35	11.26	11.04	12.40	11.37	12.13	11.95	11.84	11.82	11.46
B (Boron atom)	5.01	4.10	3.50	2.97	3.80	4.14	3.82	3.75	3.69	3.66
BCl3 (Borane, trichloro-)	7.48	6.40	6.46	7.05	6.88	7.61	7.42	7.21	7.16	7.01
Be (Beryllium atom)	5.33	4.88	4.90	5.10	4.88	4.98	4.90	4.88	4.75	4.37
BF3 (Borane, trifluoro-)	12.80	10.85	10.46	10.74	11.44	12.05	12.08	11.87	12.37	12.95
C (Carbon atom)	7.64	5.92	5.28	4.77	5.82	6.12	5.71	5.64	5.89	6.01
C2F4 (Tetrafluoroethylene)	7.14	6.12	5.77	6.20	6.26	7.02	6.97	6.77	6.61	6.85
C2H2 (Acetylene)	8.41	7.50	7.06	7.33	7.30	8.31	8.12	7.71	7.67	7.69
C2H2O2 (Ethanedial)	3.00	2.05	2.15	2.56	2.53	2.85	2.78	2.68	2.54	2.05
C2H4 (Ethylene)	7.42	6.84	6.45	6.78	6.60	7.55	7.38	7.02	6.92	6.87
C2H4O (Ethylene oxide)	7.48	6.20	5.88	6.30	6.65	7.70	7.62	7.26	7.51	7.82
C2H4S (Thiirane)	6.02	5.13	4.87	5.71	5.28	6.42	6.24	5.92	5.74	5.72
C2H5N (Aziridine)	6.37	5.49	5.25	5.70	5.72	6.74	6.59	6.24	6.15	6.39
C2H6 (Ethane)	10.09	8.59	8.34	8.82	8.92	10.02	9.87	9.43	9.36	9.61
C2HF3 (Trifluoroethylene)	6.86	5.98	5.64	6.00	6.05	6.70	6.67	6.49	6.33	6.26
C2N2 (Cyanogen)	8.32	6.86	6.99	7.48	7.67	8.46	8.34	8.12	7.97	7.97
C3H4 (Cyclopropene)	6.78	5.96	5.89	6.19	6.14	6.47	6.42	6.33	6.31	6.09
C3H6 (Cyclopropane)	8.46	7.12	6.76	7.12	7.13	8.28	8.10	7.69	8.01	7.47
C3H8 (Propane)	8.93	7.44	7.30	7.88	7.89	8.98	8.80	8.42	8.28	8.54
C3O2 (Carbon suboxide)	7.25	7.07	6.70	7.17	6.90	7.52	7.44	7.26	7.11	6.93
C4H2 (Diacetylene)	8.06	7.08	6.60	6.81	6.88	8.16	8.01	7.54	7.33	7.53
C4H4O (Furan)	6.47	6.00	5.75	5.91	5.95	6.23	6.19	6.12	6.15	6.21
C4H6 (Cyclobutene)	6.77	5.99	5.66	5.99	5.93	7.04	6.86	6.47	6.31	6.41
C4N2 (2-Butynedinitrile)	8.25	6.02	6.19	6.74	7.21	8.47	8.31	7.99	7.91	8.10
CCl4 (Carbon tetrachloride)	7.27	5.07	6.06	6.43	6.73	7.24	7.16	7.04	6.88	6.61
CF2Cl2 (Difluorodichloromethane)	7.43	6.43	6.45	6.99	6.85	7.38	7.29	7.17	7.05	6.76
CF2O (Carbonic difluoride)	9.50	8.16	7.83	8.51	8.59	9.39	9.37	9.17	9.38	9.84
CF3Br (Bromotrifluoromethane)	8.99	6.17	6.19	6.59	6.28	6.47	8.81	8.53	8.43	8.41
CF3Cl (Methane, chlorotrifluoro-)	9.96	7.67	7.67	8.30	7.83	9.96	9.77	8.01	9.38	9.41
CF4 (Carbon tetrafluoride)	13.82	11.81	11.22	11.49	12.37	13.07	13.13	12.77	13.35	14.18
CFCl3 (Trichloromonofluoromethane)	7.12	5.83	5.85	6.31	6.42	7.08	6.98	6.82	6.74	6.56
CH2CCH2 (Allene)	7.13	6.50	6.15	6.50	6.41	7.39	7.21	6.87	6.74	6.79

CH2CCl2 (Ethene, 1,1-dichloro-)	6.82	5.98	5.93	5.89	6.14	6.57	6.49	6.38	6.38	6.39
CH2CF2 (Ethene, 1,1-difluoro-)	7.32	6.49	6.09	6.45	6.44	7.34	7.22	6.90	6.81	6.93
CH2CHCHO (Acrolein)	3.90	3.04	3.12	3.53	3.54	3.89	3.83	3.73	3.56	3.10
CH2CHCl (Ethene, chloro-)	6.98	6.08	6.01	6.39	6.25	6.85	6.77	6.65	6.57	6.54
CH2CHF (Ethene, fluoro-)	7.36	6.60	6.19	6.53	6.47	7.43	7.28	6.91	6.82	6.86
CH2Cl2 (Methylene chloride)	7.23	6.10	6.11	6.61	6.57	7.19	7.09	6.94	6.82	6.72
CH2CO (Ketene)	6.12	5.71	5.35	5.76	5.60	6.35	6.23	5.98	5.84	5.75
CH2F2 (Methane, difluoro-)	9.75	8.06	7.73	8.16	8.53	9.38	9.33	8.97	9.17	9.80
CH3 (Methyl radical)	5.91	5.10	4.92	5.24	5.20	5.89	5.78	5.45	5.34	4.83
CH3CCCH3 (2-Butyne)	6.74	5.69	5.39	5.81	5.75	6.87	6.68	6.32	6.16	6.24
CH3CCH (Propyne)	7.42	6.32	5.99	6.37	6.34	6.86	6.84	6.80	6.78	6.87
CH3CH2Cl (Ethyl chloride)	7.55	6.54	6.35	6.86	6.86	7.56	7.47	7.33	7.14	6.96
CH3CH2OH (Ethanol)	6.83	5.77	5.52	6.02	6.13	6.94	6.84	6.57	6.65	6.86
CH3Cl (Methyl chloride)	7.44	6.55	6.37	6.90	6.77	7.49	7.39	7.23	7.03	6.87
CH3COCl (Acetyl Chloride)	7.36	4.93	4.97	5.47	6.59	7.17	6.94	6.63	6.80	7.22
CH3F (Methyl fluoride)	9.60	8.01	7.68	8.16	8.48	9.26	9.24	8.94	9.16	9.45
CH3NHCH3 (Dimethylamine)	5.68	4.73	4.52	5.05	5.04	6.04	5.88	5.54	5.49	5.67
CH3NO2 (Methane, nitro-)	4.75	3.92	3.95	4.35	6.80	6.81	6.84	6.86	6.72	6.38
CH3OCH3 (Dimethyl ether)	6.88	5.59	5.34	5.86	6.05	7.10	6.97	6.62	6.80	7.34
CH3OH (Methyl alcohol)	6.90	5.88	5.62	6.12	6.20	6.96	6.86	6.61	6.71	6.89
CH3SH (Methanethiol)	5.57	4.93	4.77	5.29	5.04	5.69	5.60	5.45	5.20	4.96
CH3SiH3 (Methyl silane)	8.48	7.48	7.37	7.89	7.77	8.78	8.59	8.27	7.98	7.92
CH4 (Methane)	10.67	9.40	9.14	9.68	9.62	10.52	10.35	9.98	9.97	10.10
CHCl3 (Chloroform)	7.19	6.05	6.06	6.55	6.60	7.20	7.11	6.97	6.85	6.63
CHF3 (Methane, trifluoro-)	11.14	9.41	9.03	9.38	9.85	10.67	10.63	10.26	10.52	11.21
CHONH2 (Formamide)	5.74	5.35	5.29	5.76	5.57	5.70	5.67	5.64	5.45	4.97
Cl (Chlorine atom)	9.43	8.65	8.50	9.58	8.76	9.54	9.40	9.22	8.91	8.12
Cl2 (Chlorine diatomic)	3.95	3.41	3.47	3.83	3.59	3.86	3.79	3.71	3.59	3.42
ClF (Chlorine monofluoride)	4.38	7.77	7.76	4.37	8.18	4.12	8.54	8.42	3.97	3.53
ClF3 (Chlorine trifluoride)	4.57	3.47	3.53	3.98	3.98	4.26	4.24	4.18	4.32	4.17
ClO (Monochlorine monoxide)	4.93	4.57	4.47	5.00	4.71	4.79	4.84	4.88	4.62	4.33
CO (Carbon monoxide)	8.62	8.19	8.24	8.61	8.39	8.57	8.52	8.47	8.20	7.86
CO2 (Carbon dioxide)	11.27	10.52	9.96	10.14	10.51	11.18	11.14	10.74	10.97	11.36
CS (Carbon monosulfide)	4.96	4.63	4.70	4.95	4.76	4.90	4.87	4.83	4.39	3.80
CS2 (Carbon disulfide)	6.55	6.55	6.46	7.44	6.51	3.70	3.73	3.82	7.47	7.23
F (Fluorine atom)	13.68	12.29	11.99	13.12	12.60	12.89	13.08	13.13	13.21	12.95
F2 (Fluorine diatomic)	4.67	4.15	4.25	4.87	4.36	4.46	4.43	4.42	4.11	12.74
F2O (Difluorine monoxide)	7.43	6.99	7.04	7.57	7.26	7.45	7.43	7.41	7.31	6.44

FCN (Cyanogen fluoride)	8.38	7.64	7.41	8.09	7.65	8.18	8.12	8.02	7.93	7.58
H (Hydrogen atom)	10.86	9.38	9.63	10.47	9.86	9.92	9.88	9.86	10.16	10.50
H2CO (Formaldehyde)	7.28	6.12	5.81	6.28	6.47	7.40	7.31	6.93	7.12	7.65
H2CS (Thioformaldehyde)	6.01	5.30	5.03	5.43	5.37	6.22	6.23	5.90	5.72	5.84
H2O (Water)	7.67	6.72	6.42	6.94	6.93	7.57	7.48	7.26	7.46	7.58
H2O2 (Hydrogen peroxide)	5.76	5.23	5.22	5.82	5.42	5.68	5.63	5.59	5.32	4.51
H2S (Hydrogen sulfide)	6.38	5.76	5.56	6.16	5.76	6.61	6.42	6.16	6.00	5.79
HCCCN (Cyanoacetylene)	8.49	6.88	7.02	7.57	7.62	8.57	8.41	8.08	7.97	7.94
HCCF (Fluoroacetylene)	7.55	6.72	6.40	6.83	6.67	7.40	7.30	7.08	7.00	6.83
HCl (Hydrogen sulfide)	7.96	7.29	7.10	7.76	7.32	8.00	7.87	7.69	7.54	7.28
HCN (Hydrogen cyanide)	9.25	8.65	8.68	8.98	8.99	9.40	9.33	9.24	8.96	8.65
HCO (Formyl radical)	2.22	2.04	2.22	2.55	2.32	2.29	2.28	2.29	1.92	1.17
HCOOH (Formic acid)	5.69	5.38	5.42	5.86	5.54	5.67	5.63	5.60	5.38	4.80
He (Helium atom)	24.04	21.89	22.13	23.63	22.76	22.46	22.64	22.93	23.23	23.52
HF (Hydrogen fluoride)	10.50	9.16	8.79	9.34	9.47	9.96	9.98	9.81	10.16	10.35
Li (Lithium atom)	1.84	1.99	1.99	2.05	1.98	1.98	1.87	1.83	1.94	2.23
Mg (Magnesium atom)	4.29	4.31	4.18	4.25	4.23	4.27	4.25	4.25	4.35	4.25
N (Nitrogen atom)	10.51	9.14	8.76	10.05	9.39	9.70	9.79	9.70	10.08	9.89
N2 (Nitrogen diatomic)	13.25	11.72	11.26	11.53	12.12	12.95	12.87	12.47	12.74	12.81
N2H4 (Hydrazine)	5.62	4.53	4.36	4.99	4.89	5.87	5.70	5.39	5.40	5.71
N2O (Nitrous oxide)	8.68	8.31	7.96	9.52	9.59	9.98	9.98	9.84	9.79	8.03
Na (Sodium atom)	2.02	2.29	2.13	1.64	2.24	1.85	1.89	1.92	2.53	2.97
NaCl (Sodium Chloride)	4.97	3.39	3.03	3.40	3.46	5.16	4.98	4.47	4.03	4.29
Ne (Neon atom)	18.12	16.22	15.85	17.16	16.63	16.67	17.00	17.25	17.59	18.04
NF3 (Nitrogen trifluoride)	9.22	7.66	7.73	8.48	8.22	8.52	8.54	8.48	8.58	8.14
NH (Imidogen)	3.74	3.62	3.98	4.22	3.88	3.79	3.81	3.86	3.32	2.25
NH2 (Amino radical)	2.12	1.98	2.36	2.77	2.27	2.17	2.17	2.22	1.67	0.82
NH3 (Ammonia)	6.65	5.78	5.52	6.06	5.94	6.75	6.59	6.30	6.41	6.58
NO (Nitric oxide)	6.25	5.13	4.85	4.99	5.63	6.18	6.19	5.93	6.05	6.26
NO2 (Nitrogen dioxide)	2.96	2.84	2.96	3.14	2.96	2.96	2.94	2.93	2.61	2.01
O (Oxygen atom)	9.99	8.99	8.97	9.90	9.35	9.85	9.83	9.69	9.25	8.27
O2 (Oxygen diatomic)	8.84	8.08	7.64	7.84	8.52	8.59	8.57	8.57	8.56	8.17
O3 (Ozone)	5.28	5.27	5.21	5.23	5.02	4.90	4.93	4.99	4.85	4.56
OCS (Carbonyl sulfide)	7.54	7.18	6.94	7.69	7.11	7.80	7.67	7.49	7.26	6.80
OH (Hydroxyl radical)	4.13	3.83	4.30	4.96	4.21	4.17	4.17	4.20	3.59	2.16
P (Phosphorus atom)	7.09	6.22	6.07	7.16	6.31	7.01	6.88	6.60	6.69	6.27
P2 (Phosphorus diatomic)	6.66	6.16	6.10	6.24	6.10	6.20	6.21	6.20	6.18	6.10
PF3 (Phosphorus trifluoride)	8.10	7.44	7.26	7.61	7.60	7.91	7.89	7.80	7.68	7.53

PH3 (Phosphine)	6.96	6.27	6.10	6.64	6.34	7.18	7.01	6.74	6.54	6.32
S (Sulfur atom)	7.00	6.56	6.46	7.23	6.58	7.36	7.19	6.96	6.22	4.94
S2 (Sulfur diatomic)	4.75	4.47	4.51	4.64	4.69	4.46	4.55	4.63	4.66	4.60
Si (Silicon atom)	4.99	4.39	4.29	4.95	4.44	5.05	4.94	4.68	4.59	4.36
Si2H6 (Disilane)	7.62	7.08	6.93	7.40	7.28	7.63	7.56	7.49	7.30	7.20
SiF2 (Silicon difluoride)	5.67	5.35	5.31	5.55	5.48	5.51	5.51	5.48	5.45	5.23
SiF4 (Silicon tetrafluoride)	13.27	10.89	10.63	11.31	11.71	12.49	12.48	12.28	12.74	13.38
SiH3 (Silyl)	5.42	4.64	4.78	5.10	4.95	5.00	5.00	5.07	4.90	3.19
SiH4 (Silane)	9.49	8.29	8.13	8.78	8.57	9.50	9.32	8.97	8.84	8.67
SiO (Silicon monoxide)	5.62	5.25	5.19	5.48	5.39	5.65	5.59	5.51	5.47	5.49
SO2 (Sulfur dioxide)	4.44	4.14	4.12	4.29	4.17	4.28	4.25	4.20	4.03	3.67
MAE		0.97	1.12	0.70	0.76	0.31	0.32	0.46	0.46	0.68
MSE		-0.91	-1.05	-0.61	-0.63	-0.13	-0.15	-0.33	-0.38	-0.44
RMS		1.15	1.29	0.90	0.92	0.55	0.63	0.71	0.54	1.05

Table S10. Exciton binding energies (1) [in eV] of the 121 molecules studied. The reference values are the differences between the CCSD fundamental gaps and the EOM-CCSD optical gaps.

Molecule	Ref.	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	2.39	2.66	2.76	2.40	2.79	2.41	2.45	2.63	2.80	3.22
AlCl3 (Aluminum trichloride)	4.11	4.24	4.05	4.11	4.04	4.36	4.31	4.20	4.36	4.52
Ar (Argon atom)	6.14	7.30	7.25	6.54	6.99	6.54	6.67	6.67	6.50	6.46
B (Boron atom)	3.01	3.86	4.55	5.37	4.48	4.13	4.45	4.45	4.38	4.30
BCl3 (Borane, trichloro-)	4.74	4.59	4.36	4.27	4.41	4.52	4.50	4.49	4.66	5.08
Be (Beryllium atom)	4.34	4.21	4.09	4.04	4.30	4.38	4.32	4.20	4.61	5.08
BF3 (Borane, trifluoro-)	4.58	4.59	4.58	4.59	4.41	4.64	4.44	4.48	4.51	4.75
C (Carbon atom)	2.38	3.99	4.68	5.32	4.35	4.03	4.45	4.48	4.16	4.05
C2F4 (Tetrafluoroethylene)	4.84	5.11	5.09	5.47	5.03	4.66	4.73	4.85	5.22	5.74
C2H2 (Acetylene)	4.92	4.84	4.73	4.30	4.48	3.60	3.82	4.21	4.32	5.82
C2H2O2 (Ethanedial)	7.23	6.92	6.78	6.66	6.88	7.05	7.03	6.99	7.33	8.31
C2H4 (Ethylene)	4.90	4.73	4.62	4.29	4.57	3.57	3.76	4.27	4.35	5.37
C2H4O (Ethylene oxide)	4.06	5.04	4.97	4.80	4.39	3.61	3.66	3.93	4.04	3.95
C2H4S (Thiirane)	3.79	4.61	4.49	3.93	4.23	3.25	3.44	3.69	4.10	4.19
C2H5N (Aziridine)	3.98	4.84	4.73	4.55	4.42	3.66	3.77	4.03	4.31	3.95
C2H6 (Ethane)	3.37	3.89	3.98	4.06	3.83	3.23	3.31	3.59	3.78	3.53
C2HF3 (Trifluoroethylene)	4.19	4.83	4.71	5.49	4.63	4.11	4.17	4.30	5.71	6.10
C2N2 (Cyanogen)	5.48	6.32	6.00	5.63	5.36	4.87	4.92	5.08	5.50	5.72
C3H4 (Cyclopropene)	4.88	4.56	4.25	4.99	4.13	3.96	4.01	4.03	4.18	5.70
C3H6 (Cyclopropane)	3.09	4.46	4.42	4.36	4.18	3.32	3.47	3.81	3.56	3.84
C3H8 (Propane)	3.90	4.16	4.18	4.13	4.10	3.65	3.73	3.91	4.14	3.98
C3O2 (Carbon suboxide)	4.10	4.63	4.82	4.43	4.53	4.18	4.28	4.43	4.66	4.56
C4H2 (Diacetylene)	3.42	3.75	3.97	4.05	3.82	2.52	2.66	3.44	3.85	3.92
C4H4O (Furan)	3.20	3.71	3.51	3.48	3.35	3.28	3.32	3.33	4.36	4.53
C4H6 (Cyclobutene)	5.09	4.19	4.14	4.24	3.95	3.04	3.22	3.56	4.36	5.56
C4N2 (2-Butynedinitrile)	3.22	4.53	4.23	3.83	3.35	2.47	2.56	2.78	3.13	3.23
CCl4 (Carbon tetrachloride)	5.03	5.35	4.25	4.44	4.20	5.11	4.91	4.62	5.00	6.03
CF2Cl2 (Difluorodichloromethane)	5.89	5.72	5.47	5.56	5.56	6.13	6.04	5.87	6.11	6.47
CF2O (Carbonic difluoride)	6.47	6.19	6.09	5.91	5.67	5.30	5.29	5.40	5.79	5.74
CF3Br (Bromotrifluoromethane)	3.84	6.25	5.91	5.70	6.14	6.34	3.95	4.11	4.26	4.58
CF3Cl (Methane, chlorotrifluoro-)	4.18	5.96	5.62	5.62	5.91	4.26	4.40	6.06	4.83	4.66
CF4 (Carbon tetrafluoride)	4.30	4.14	4.34	4.95	4.17	4.28	4.19	4.35	4.39	4.52
CFCl3 (Trichloromonofluoromethane)	5.53	5.23	5.05	5.25	5.02	5.66	5.52	5.32	5.60	6.40
CH2CCH2 (Allene)	3.59	4.37	4.30	4.16	4.12	3.31	3.50	3.80	4.32	3.81
CH2CCl2 (Ethene, 1,1-dichloro-)	4.15	4.53	3.97	4.71	3.98	3.98	4.00	3.99	4.11	4.03

CH2CF2 (Ethene, 1,1-difluoro-)	4.32	4.73	4.65	4.39	4.52	3.75	3.90	4.17	4.43	5.58
CH2CHCHO (Acrolein)	6.68	6.83	6.63	6.39	6.39	6.27	6.27	6.32	6.65	7.33
CH2CHCl (Ethene, chloro-)	4.00	5.03	4.22	4.72	4.11	3.81	3.85	3.87	4.80	5.03
CH2CHF (Ethene, fluoro-)	4.03	4.65	4.59	5.25	5.34	3.57	3.74	4.06	5.32	5.55
CH2Cl2 (Methylene chloride)	4.95	5.09	4.88	4.93	5.02	5.10	5.08	5.03	5.29	5.33
CH2CO (Ketene)	4.08	4.83	4.77	4.42	4.57	3.97	4.09	4.30	4.83	5.25
CH2F2 (Methane, difluoro-)	4.53	5.05	5.07	5.03	4.90	4.39	4.42	4.65	4.87	4.73
CH3 (Methyl radical)	4.04	4.63	5.05	4.84	4.71	4.04	4.12	4.42	4.52	4.83
CH3CCCH3 (2-Butyne)	3.57	4.23	4.20	3.96	4.60	3.21	3.40	3.69	4.04	4.33
CH3CCH (Propyne)	3.52	4.62	4.56	4.35	4.33	3.98	4.00	3.99	4.12	4.36
CH3CH2Cl (Ethyl chloride)	4.09	5.09	4.63	4.72	4.45	4.14	4.20	4.23	4.52	4.48
CH3CH2OH (Ethanol)	4.45	4.98	4.98	4.85	4.75	4.32	4.37	4.52	4.63	4.44
CH3Cl (Methyl chloride)	4.46	5.14	5.04	4.89	4.87	4.47	4.54	4.62	4.93	5.81
CH3COCl (Acetyl Chloride)	4.78	6.35	6.01	5.81	4.64	4.45	4.63	4.83	5.04	5.55
CH3F (Methyl fluoride)	4.44	5.40	5.42	5.23	5.02	4.53	4.52	4.72	4.76	4.66
CH3NHCH3 (Dimethylamine)	3.87	4.68	4.59	4.32	4.28	3.60	3.73	3.96	4.11	3.96
CH3NO2 (Methane, nitro-)	6.94	7.28	6.98	6.84	4.59	5.37	5.27	5.08	5.34	6.09
CH3OCH3 (Dimethyl ether)	3.81	4.81	4.75	4.52	4.31	3.60	3.69	3.94	3.90	3.29
CH3OH (Methyl alcohol)	4.67	5.47	5.40	5.09	5.07	4.61	4.66	4.81	4.91	4.79
CH3SH (Methanethiol)	4.33	4.93	4.79	4.68	4.68	4.30	4.40	4.49	4.77	4.79
CH3SiH3 (Methyl silane)	3.78	4.27	4.21	4.13	4.17	4.04	4.15	4.30	4.21	4.49
CH4 (Methane)	4.34	5.28	5.26	5.11	5.04	4.35	4.50	4.80	4.94	4.79
CHCl3 (Chloroform)	4.99	4.85	4.68	4.78	4.66	5.09	4.99	4.83	5.12	5.44
CHF3 (Methane, trifluoro-)	4.44	4.90	4.92	4.92	4.80	4.36	4.37	5.51	4.76	4.69
CHONH2 (Formamide)	4.93	5.47	5.12	5.83	4.95	5.01	5.00	4.94	6.56	7.29
Cl (Chlorine atom)	-0.11	0.77	0.82	-0.30	0.64	-0.15	-0.02	0.17	0.48	1.32
Cl2 (Chlorine diatomic)	7.05	7.00	6.83	6.90	6.93	7.10	7.09	7.08	7.35	7.61
ClF (Chlorine monofluoride)	8.09	4.18	4.03	7.83	3.88	8.17	3.74	3.86	8.57	9.19
ClF3 (Chlorine trifluoride)	7.48	7.58	7.40	7.29	7.38	7.44	7.44	7.45	7.68	8.30
ClO (Monochlorine monoxide)	4.07	4.31	4.33	3.92	4.27	4.21	4.17	4.13	4.35	4.74
CO (Carbon monoxide)	6.87	6.89	6.53	6.22	6.79	7.13	7.12	6.90	7.24	8.12
CO2 (Carbon dioxide)	3.34	4.22	4.35	4.75	3.95	3.72	3.70	4.01	3.92	3.66
CS (Carbon monosulfide)	6.47	6.75	6.49	6.27	6.57	7.77	7.72	6.56	7.04	7.84
CS2 (Carbon disulfide)	3.35	3.66	3.54	2.83	3.40	7.53	6.12	6.12	2.62	2.71
F (Fluorine atom)	0.40	1.61	2.02	1.01	1.61	1.13	1.00	1.00	1.01	1.21
F2 (Fluorine diatomic)	10.99	10.71	10.43	10.20	10.76	10.73	10.83	10.88	11.64	3.41
F2O (Difluorine monoxide)	6.50	5.94	5.73	5.64	6.06	6.10	6.16	6.18	6.77	8.20
FCN (Cyanogen fluoride)	5.83	6.48	6.32	6.13	6.22	5.99	6.04	6.08	6.35	6.79

H (Hydrogen atom)	2.01	2.81	3.27	2.65	2.90	3.08	3.03	3.01	2.80	2.38
H2CO (Formaldehyde)	4.16	5.32	5.43	5.22	4.83	4.45	4.11	4.74	4.69	4.42
H2CS (Thioformaldehyde)	3.05	3.70	3.80	3.55	3.49	2.62	2.64	3.02	3.32	3.37
H2O (Water)	5.54	6.96	6.76	6.29	6.28	5.84	5.87	6.01	5.90	5.83
H2O2 (Hydrogen peroxide)	6.95	6.82	6.48	6.24	6.79	6.79	6.80	6.73	7.46	8.70
H2S (Hydrogen sulfide)	4.50	5.31	5.17	4.97	5.05	4.41	4.61	4.83	5.02	5.05
HCCCN (Cyanoacetylene)	3.58	4.93	4.54	4.18	4.06	3.47	3.49	3.83	4.17	4.44
HCCF (Fluoroacetylene)	4.36	5.26	5.11	5.91	4.98	4.37	4.50	4.68	6.11	6.54
HCl (Hydrogen sulfide)	5.26	6.14	5.95	5.66	5.82	5.37	5.49	5.62	5.84	6.00
HCN (Hydrogen cyanide)	4.86	5.99	5.41	5.79	5.06	4.63	4.71	4.78	6.13	6.75
HCO (Formyl radical)	7.51	7.54	7.49	7.25	7.61	7.67	7.66	7.64	7.95	8.82
HCOOH (Formic acid)	6.15	6.54	6.03	6.41	6.09	6.21	6.21	6.14	7.45	8.47
He (Helium atom)	3.16	4.95	4.66	3.70	4.55	4.84	4.61	4.28	3.96	3.50
HF (Hydrogen fluoride)	6.27	8.19	7.97	7.37	7.31	6.97	6.87	6.96	6.70	6.53
Li (Lithium atom)	2.89	2.96	3.08	2.53	3.09	2.95	2.95	3.03	2.94	3.19
Mg (Magnesium atom)	3.48	3.53	3.45	3.48	3.57	3.70	3.63	3.44	3.68	3.72
N (Nitrogen atom)	4.29	5.51	5.69	4.84	5.03	4.90	4.86	4.99	4.59	4.44
N2 (Nitrogen diatomic)	4.78	5.58	5.78	5.71	5.17	4.84	4.89	5.16	5.03	6.08
N2H4 (Hydrazine)	4.68	5.35	5.29	5.16	5.06	4.42	4.53	4.72	4.94	4.74
N2O (Nitrous oxide)	6.14	6.01	5.91	5.23	4.33	4.27	4.25	4.35	5.04	6.68
Na (Sodium atom)	2.12	2.53	2.68	2.37	2.61	2.49	2.42	2.53	2.08	2.12
NaCl (Sodium Chloride)	3.51	5.52	5.49	5.43	5.05	3.45	3.65	4.13	4.64	4.09
Ne (Neon atom)	8.66	10.93	10.73	9.49	9.98	10.42	9.90	9.56	8.79	8.21
NF3 (Nitrogen trifluoride)	6.55	6.95	6.55	6.49	6.64	6.87	6.83	6.76	6.83	7.41
NH (Imidogen)	9.56	9.53	9.25	9.16	9.34	9.47	9.46	9.43	9.99	11.02
NH2 (Amino radical)	9.30	9.21	8.97	8.58	9.24	9.35	9.26	9.19	9.62	10.38
NH3 (Ammonia)	4.77	5.99	5.82	5.38	5.47	4.84	4.96	5.18	5.15	4.96
NO (Nitric oxide)	3.97	5.04	5.17	5.20	4.70	4.11	4.14	4.40	4.34	4.40
NO2 (Nitrogen dioxide)	7.14	7.04	7.01	7.08	7.30	7.29	7.33	7.37	7.73	8.54
O (Oxygen atom)	2.23	3.01	3.32	2.48	3.11	2.48	2.49	2.64	3.01	4.16
O2 (Oxygen diatomic)	3.91	4.59	5.02	5.23	4.45	4.36	4.41	4.46	4.58	4.96
O3 (Ozone)	5.71	5.57	5.49	5.46	5.69	5.84	5.80	5.75	6.05	6.70
OCS (Carbonyl sulfide)	4.53	5.35	5.30	4.84	4.89	4.46	4.59	4.74	5.33	5.69
OH (Hydroxyl radical)	7.24	7.39	7.03	6.45	7.28	7.24	7.24	7.22	7.84	9.14
P (Phosphorus atom)	2.74	3.30	3.54	2.80	3.12	2.66	2.70	2.94	2.77	2.92
P2 (Phosphorus diatomic)	3.32	4.00	3.83	3.77	3.72	3.43	3.99	4.00	3.73	3.72
PF3 (Phosphorus trifluoride)	4.87	5.05	4.84	4.84	4.90	5.01	5.01	4.98	5.13	5.48
PH3 (Phosphine)	4.09	4.83	4.72	4.63	4.64	3.94	4.14	4.38	4.53	4.37

S (Sulfur atom)	1.26	1.65	1.80	1.00	1.78	1.01	1.15	1.37	2.10	3.38
S2 (Sulfur diatomic)	3.32	3.53	3.60	3.66	3.46	3.86	3.69	3.56	3.50	3.45
Si (Silicon atom)	1.76	2.39	2.41	1.72	2.33	1.80	1.89	2.12	2.13	2.40
Si2H6 (Disilane)	3.60	3.77	3.65	3.78	3.55	3.53	3.59	3.59	3.80	3.83
SiF2 (Silicon difluoride)	5.37	5.46	5.21	5.20	5.31	5.47	5.42	5.37	5.41	5.61
SiF4 (Silicon tetrafluoride)	4.45	4.34	4.29	4.57	4.16	4.49	4.37	4.28	4.44	4.87
SiH3 (Silyl)	2.59	3.15	3.23	3.03	3.04	2.98	2.97	2.88	3.18	4.77
SiH4 (Silane)	3.96	4.39	4.39	4.46	4.33	3.91	4.01	4.21	4.33	4.45
SiO (Silicon monoxide)	5.88	6.11	5.89	5.77	5.86	5.87	5.89	5.89	6.03	6.23
SO2 (Sulfur dioxide)	7.27	7.36	7.19	7.14	7.25	7.26	7.29	7.32	7.63	8.19
MAE		0.66	0.66	0.57	0.53	0.39	0.38	0.40	0.48	0.80
MSE		0.52	0.42	0.32	0.24	0.04	0.01	0.12	0.36	0.62
RMS		0.88	0.88	0.74	0.78	0.71	0.71	0.71	0.61	1.16

Table S11. Exciton binding energies (2) [in eV] of the 121 molecules studied. The reference values are the differences between the CCSD fundamental gaps and the EOM-CCSD optical gaps.

Molecule	Ref.	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	2.39	1.51	1.62	1.45	1.77	2.01	1.99	2.03	2.08	2.78
AlCl3 (Aluminum trichloride)	4.11	3.10	2.89	2.84	3.17	4.22	4.02	3.72	3.96	4.95
Ar (Argon atom)	6.14	3.78	3.84	3.08	4.61	5.66	5.42	4.80	5.12	6.84
B (Boron atom)	3.01	1.79	2.45	3.23	2.68	3.20	3.40	3.18	3.14	3.39
BCl3 (Borane, trichloro-)	4.74	4.02	3.33	3.13	3.99	4.07	4.08	4.13	4.52	5.27
Be (Beryllium atom)	4.34	2.18	2.02	1.96	2.58	4.20	4.05	3.68	3.41	4.77
BF3 (Borane, trifluoro-)	4.58	1.59	1.64	1.44	2.34	4.01	3.64	3.26	3.59	5.89
C (Carbon atom)	2.38	2.02	2.70	3.59	2.66	2.88	3.20	3.07	2.96	3.29
C2F4 (Tetrafluoroethylene)	4.84	2.62	2.33	2.90	3.27	4.64	4.43	4.03	4.26	6.51
C2H2 (Acetylene)	4.92	1.29	1.39	1.28	2.05	3.55	3.43	3.25	3.18	6.13
C2H2O2 (Ethanedial)	7.23	6.60	6.43	6.33	6.60	6.70	6.71	6.69	7.20	8.47
C2H4 (Ethylene)	4.90	1.68	1.74	1.51	2.39	3.70	3.58	3.55	3.45	5.85
C2H4O (Ethylene oxide)	4.06	1.77	1.82	1.73	2.37	3.62	3.44	3.19	3.45	5.75
C2H4S (Thiirane)	3.79	1.96	1.93	1.36	2.40	3.48	3.35	3.08	3.26	5.09
C2H5N (Aziridine)	3.98	1.97	1.96	1.82	2.56	3.78	3.63	3.38	3.60	5.02
C2H6 (Ethane)	3.37	1.15	1.27	1.29	1.85	3.08	2.94	2.77	2.81	4.16
C2HF3 (Trifluoroethylene)	4.19	2.06	2.04	3.15	2.68	4.09	3.87	3.50	4.95	6.77
C2N2 (Cyanogen)	5.48	5.81	5.51	5.26	5.01	4.70	4.71	4.80	5.20	5.50
C3H4 (Cyclopropene)	4.88	1.80	1.59	2.86	2.14	4.07	3.85	3.37	3.37	5.98
C3H6 (Cyclopropane)	3.09	1.68	1.73	1.68	2.32	3.55	3.43	3.25	2.75	4.65
C3H8 (Propane)	3.90	1.78	1.80	1.66	2.36	3.63	3.51	3.29	3.36	4.53
C3O2 (Carbon suboxide)	4.10	4.33	4.43	4.31	4.35	4.22	4.07	3.78	3.87	4.44
C4H2 (Diacetylene)	3.42	2.37	2.48	2.47	2.81	2.68	2.58	3.10	3.37	4.09
C4H4O (Furan)	3.20	1.28	1.19	1.24	1.71	3.57	3.36	2.92	3.80	5.14
C4H6 (Cyclobutene)	5.09	1.67	1.71	1.82	2.23	3.37	3.28	3.12	3.63	5.93
C4N2 (2-Butynedinitrile)	3.22	4.29	3.99	3.62	3.18	2.40	2.46	2.65	2.97	3.16
CCl4 (Carbon tetrachloride)	5.03	4.71	3.52	4.03	3.63	4.82	4.63	4.31	4.69	6.23
CF2Cl2 (Difluorodichloromethane)	5.89	3.94	3.64	3.60	4.23	6.03	5.73	5.21	5.40	7.26
CF2O (Carbonic difluoride)	6.47	2.96	2.96	2.84	3.60	4.95	4.68	4.26	5.10	7.28
CF3Br (Bromotrifluoromethane)	3.84	4.19	3.81	3.96	4.71	6.27	3.63	3.39	3.79	4.75
CF3Cl (Methane, chlorotrifluoro-)	4.18	3.30	3.02	3.06	3.98	4.11	3.93	5.08	3.92	5.53
CF4 (Carbon tetrafluoride)	4.30	1.32	1.57	2.06	2.19	3.77	3.51	3.25	3.56	5.71
CFCl3 (Trichloromonofluoromethane)	5.53	4.14	3.89	4.11	4.18	5.41	5.23	4.92	5.19	6.57
CH2CCH2 (Allene)	3.59	1.68	1.73	1.82	2.32	3.60	3.50	3.30	3.64	4.56
CH2CCl2 (Ethene, 1,1-dichloro-)	4.15	3.31	1.94	3.39	2.52	4.19	3.99	3.56	3.52	4.80

CH2CF2 (Ethene, 1,1-difluoro-)	4.32	1.85	1.90	1.72	2.52	3.79	3.64	3.39	3.54	6.24
CH2CHCHO (Acrolein)	6.68	5.78	5.55	5.66	5.95	6.32	6.29	6.20	6.90	8.23
CH2CHCl (Ethene, chloro-)	4.00	3.46	1.86	3.04	2.42	3.92	3.71	3.29	4.33	5.32
CH2CHF (Ethene, fluoro-)	4.03	1.72	1.78	3.09	3.77	3.61	3.49	3.29	4.71	5.98
CH2Cl2 (Methylene chloride)	4.95	3.12	2.87	2.77	3.40	4.94	4.70	4.24	4.44	6.13
CH2CO (Ketene)	4.08	2.31	2.26	2.04	2.60	3.94	3.79	3.51	3.91	5.62
CH2F2 (Methane, difluoro-)	4.53	1.86	1.92	1.94	2.60	3.94	3.75	3.49	3.83	5.54
CH3 (Methyl radical)	4.04	2.62	2.88	2.60	3.04	3.06	3.03	3.11	3.40	4.08
CH3CCCH3 (2-Butyne)	3.57	1.73	1.78	1.51	2.76	3.51	3.42	3.23	3.27	4.70
CH3CCH (Propyne)	3.52	1.82	1.82	1.86	2.27	4.11	3.83	3.29	3.13	4.76
CH3CH2Cl (Ethyl chloride)	4.09	2.07	2.05	2.04	2.56	4.15	3.91	3.44	3.65	5.32
CH3CH2OH (Ethanol)	4.45	2.03	2.03	1.87	2.73	4.24	4.06	3.70	3.94	5.72
CH3Cl (Methyl chloride)	4.46	2.29	2.24	1.92	2.85	4.37	4.13	3.67	3.94	6.56
CH3COCl (Acetyl Chloride)	4.78	4.27	3.85	3.73	3.02	4.56	4.53	4.27	4.67	5.31
CH3F (Methyl fluoride)	4.44	1.83	1.90	1.74	2.56	4.01	3.79	3.48	3.74	5.62
CH3NHCH3 (Dimethylamine)	3.87	1.89	1.88	1.68	2.46	3.78	3.65	3.39	3.48	4.68
CH3NO2 (Methane, nitro-)	6.94	5.11	4.67	4.61	3.23	5.11	4.82	4.17	5.05	5.09
CH3OCH3 (Dimethyl ether)	3.81	1.85	1.85	1.68	2.40	3.67	3.54	3.29	3.36	4.73
CH3OH (Methyl alcohol)	4.67	2.10	2.10	1.84	2.84	4.36	4.17	3.80	4.07	6.03
CH3SH (Methanethiol)	4.33	2.29	2.23	2.01	2.84	4.39	4.17	3.74	3.82	5.44
CH3SiH3 (Methyl silane)	3.78	2.01	1.81	1.59	2.39	3.75	3.64	3.38	3.41	4.80
CH4 (Methane)	4.34	1.73	1.81	1.83	2.53	4.02	3.85	3.58	3.64	5.32
CHCl3 (Chloroform)	4.99	3.46	3.22	3.17	3.59	4.98	4.71	4.24	4.57	6.28
CHF3 (Methane, trifluoro-)	4.44	1.83	1.90	1.92	2.59	3.91	3.70	3.45	3.72	5.50
CHONH2 (Formamide)	4.93	2.36	2.14	3.17	3.09	5.03	4.78	4.21	6.19	8.56
Cl (Chlorine atom)	-0.11	-0.19	-0.12	-1.25	-0.20	-0.81	-0.72	-0.59	-0.20	1.01
Cl2 (Chlorine diatomic)	7.05	6.00	5.82	6.01	6.24	6.79	6.74	6.63	6.91	7.66
ClF (Chlorine monofluoride)	8.09	2.85	2.72	6.68	2.95	7.78	3.23	3.18	7.95	9.16
ClF3 (Chlorine trifluoride)	7.48	7.10	6.86	6.90	7.03	7.15	7.15	7.14	7.41	8.18
ClO (Monochlorine monoxide)	4.07	3.62	3.63	3.15	3.65	3.72	3.64	3.56	3.84	4.51
CO (Carbon monoxide)	6.87	3.88	3.54	3.43	4.63	6.60	6.32	5.71	6.26	8.67
CO2 (Carbon dioxide)	3.34	1.05	1.27	1.67	1.88	3.22	2.97	2.79	2.87	4.42
CS (Carbon monosulfide)	6.47	5.71	5.51	5.68	6.04	7.93	7.63	6.38	6.98	8.21
CS2 (Carbon disulfide)	3.35	2.87	2.77	2.40	2.89	7.69	5.94	5.83	2.27	2.33
F (Fluorine atom)	0.40	-0.52	-0.15	-1.12	-0.28	-0.60	-0.76	-0.80	-0.42	0.51
F2 (Fluorine diatomic)	10.99	9.04	8.71	8.52	9.65	9.98	10.00	9.93	10.77	2.81
F2O (Difluorine monoxide)	6.50	4.51	4.21	4.41	5.18	5.67	5.65	5.53	6.35	8.43
FCN (Cyanogen fluoride)	5.83	3.53	3.47	3.09	4.19	5.61	5.32	4.83	5.18	7.14

H (Hydrogen atom)	2.01	-0.35	-0.33	-1.19	-0.08	0.59	0.43	0.21	0.28	0.31
H2CO (Formaldehyde)	4.16	3.06	3.09	2.93	2.57	4.13	3.56	3.98	4.22	5.22
H2CS (Thioformaldehyde)	3.05	2.87	3.02	2.98	2.95	2.53	2.43	2.67	3.03	3.46
H2O (Water)	5.54	2.56	2.58	2.33	3.47	5.06	4.81	4.35	4.79	7.26
H2O2 (Hydrogen peroxide)	6.95	3.22	2.94	2.66	4.26	6.27	6.00	5.37	6.36	10.15
H2S (Hydrogen sulfide)	4.50	2.28	2.26	2.01	2.93	4.29	4.14	3.80	3.82	5.50
HCCCN (Cyanoacetylene)	3.58	3.71	3.18	2.81	3.22	3.39	3.25	3.50	3.78	4.46
HCCF (Fluoroacetylene)	4.36	2.03	2.01	3.17	2.72	4.25	4.06	3.69	5.09	6.96
HCl (Hydrogen sulfide)	5.26	2.66	2.61	2.36	3.40	4.96	4.72	4.25	4.60	6.61
HCN (Hydrogen cyanide)	4.86	2.28	1.93	2.90	2.56	4.29	4.02	3.49	5.03	7.16
HCO (Formyl radical)	7.51	5.76	5.53	5.27	6.18	6.79	6.69	6.47	7.07	8.56
HCOOH (Formic acid)	6.15	3.14	2.74	3.70	3.93	6.07	5.83	5.25	6.95	9.76
He (Helium atom)	3.16	-1.93	-2.18	-2.76	-0.84	1.30	0.83	-0.13	1.03	3.65
HF (Hydrogen fluoride)	6.27	2.80	2.86	2.66	3.86	5.41	5.10	4.61	5.41	8.28
Li (Lithium atom)	2.89	2.10	2.09	2.12	2.24	2.68	2.72	2.68	2.33	2.50
Mg (Magnesium atom)	3.48	1.55	1.45	1.40	1.87	3.40	3.34	3.04	2.54	3.54
N (Nitrogen atom)	4.29	2.38	2.63	1.69	2.68	3.05	2.91	2.85	3.11	4.35
N2 (Nitrogen diatomic)	4.78	2.92	3.00	2.82	2.30	4.04	3.80	3.50	3.52	5.92
N2H4 (Hydrazine)	4.68	2.51	2.51	2.30	3.12	4.28	4.13	3.82	4.10	5.65
N2O (Nitrous oxide)	6.14	2.84	2.83	2.98	2.24	3.83	3.57	3.15	4.33	6.62
Na (Sodium atom)	2.12	1.70	1.74	2.14	1.80	2.30	2.35	2.31	1.75	1.79
NaCl (Sodium Chloride)	3.51	2.93	3.04	2.74	3.37	3.41	3.27	3.23	3.88	4.95
Ne (Neon atom)	8.66	5.12	5.18	4.39	6.30	7.40	6.90	6.20	7.35	9.82
NF3 (Nitrogen trifluoride)	6.55	4.03	3.67	3.46	4.57	6.44	6.13	5.55	5.83	8.73
NH (Imidogen)	9.56	7.06	6.73	6.74	7.43	8.00	7.91	7.72	8.74	10.42
NH2 (Amino radical)	9.30	7.61	7.33	7.04	7.87	8.33	8.22	8.04	8.88	10.27
NH3 (Ammonia)	4.77	2.24	2.26	2.14	3.02	4.49	4.31	3.94	4.09	5.97
NO (Nitric oxide)	3.97	3.25	3.37	3.37	3.40	3.25	3.21	3.33	3.54	4.16
NO2 (Nitrogen dioxide)	7.14	5.79	5.69	5.90	6.35	6.60	6.59	6.54	7.14	8.39
O (Oxygen atom)	2.23	0.92	1.10	0.48	1.23	0.90	0.86	0.93	1.70	3.02
O2 (Oxygen diatomic)	3.91	2.94	3.34	3.72	3.17	3.33	3.35	3.32	3.78	4.61
O3 (Ozone)	5.71	5.03	4.95	5.03	5.25	5.43	5.39	5.33	5.37	4.95
OCS (Carbonyl sulfide)	4.53	3.70	3.57	3.15	3.15	4.36	4.21	3.90	4.76	5.36
OH (Hydroxyl radical)	7.24	5.61	5.22	4.66	5.74	5.93	5.88	5.79	6.76	8.80
P (Phosphorus atom)	2.74	1.81	2.00	1.25	1.92	2.04	1.96	1.99	1.96	2.59
P2 (Phosphorus diatomic)	3.32	3.20	3.09	3.26	3.18	3.40	3.37	3.33	3.40	3.40
PF3 (Phosphorus trifluoride)	4.87	2.41	2.25	2.22	2.96	4.84	4.56	4.04	4.16	5.98
PH3 (Phosphine)	4.09	2.06	2.04	1.94	2.64	3.92	3.81	3.55	3.52	4.98

S (Sulfur atom)	1.26	0.68	0.81	0.13	0.90	0.39	0.48	0.62	1.41	2.90
S2 (Sulfur diatomic)	3.32	2.90	2.93	3.00	2.91	3.51	3.31	3.12	3.13	3.36
Si (Silicon atom)	1.76	1.38	1.44	0.91	1.48	1.35	1.39	1.50	1.48	1.98
Si2H6 (Disilane)	3.60	1.54	1.45	1.65	1.93	3.83	3.65	3.20	3.04	4.72
SiF2 (Silicon difluoride)	5.37	3.95	3.74	3.72	4.21	5.11	5.02	4.80	4.92	5.88
SiF4 (Silicon tetrafluoride)	4.45	2.08	2.03	2.11	2.56	4.07	3.83	3.39	3.59	5.70
SiH3 (Silyl)	2.59	2.08	2.04	1.95	2.09	2.59	2.48	2.23	2.39	4.32
SiH4 (Silane)	3.96	1.75	1.77	1.86	2.36	3.80	3.66	3.42	3.40	5.12
SiO (Silicon monoxide)	5.88	4.36	4.18	4.07	4.74	5.66	5.58	5.36	5.59	6.80
SO2 (Sulfur dioxide)	7.27	6.70	6.49	6.62	6.84	6.97	7.00	7.00	7.43	8.23
MAE		1.77	1.85	1.86	1.42	0.53	0.66	0.87	0.57	1.17
MSE		-1.74	-1.83	-1.82	-1.39	-0.34	-0.56	-0.79	-0.43	0.93
RMS		2.05	2.13	2.12	1.66	0.81	0.92	1.11	0.71	1.49

Table S12. Exciton binding energies (3) [in eV] of the 121 molecules studied. The reference values are the differences between the CCSD fundamental gaps and the EOM-CCSD optical gaps.

Molecule	Ref.	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
Al (Aluminum atom)	2.39	-2.68	-2.40	-2.39	-1.25	2.64	2.45	2.10	0.37	-0.43
AlCl3 (Aluminum trichloride)	4.11	-0.75	-0.72	-0.64	0.39	4.45	4.29	3.79	2.31	4.77
Ar (Argon atom)	6.14	-0.05	-0.10	-0.02	1.22	5.98	5.91	5.16	3.44	6.16
B (Boron atom)	3.01	-3.91	-2.95	-1.36	-1.32	3.90	3.78	2.92	1.06	0.00
BCl3 (Borane, trichloro-)	4.74	-1.52	-1.47	-1.46	-0.01	4.99	4.62	3.86	2.41	5.41
Be (Beryllium atom)	4.34	-1.36	-1.31	-1.10	0.01	4.30	4.19	3.65	1.98	4.01
BF3 (Borane, trifluoro-)	4.58	-1.26	-1.20	-0.75	0.00	4.11	3.99	3.45	2.00	5.00
C (Carbon atom)	2.38	-5.85	-4.76	-3.34	-2.77	3.25	3.04	1.95	0.24	1.67
C2F4 (Tetrafluoroethylene)	4.84	-0.24	-0.06	0.01	1.03	4.81	4.74	4.25	2.67	4.91
C2H2 (Acetylene)	4.92	-0.70	-0.27	-0.01	0.83	3.74	3.70	3.49	2.11	3.94
C2H2O2 (Ethanedial)	7.23	-0.24	-0.21	-0.08	1.65	7.08	6.67	5.78	4.81	9.36
C2H4 (Ethylene)	4.90	-1.23	-0.83	-0.73	0.66	3.90	3.88	3.59	2.19	3.98
C2H4O (Ethylene oxide)	4.06	0.01	0.01	-0.01	0.82	3.83	3.76	3.43	2.13	4.54
C2H4S (Thiirane)	3.79	-0.74	-0.46	-0.85	0.72	3.71	3.70	3.35	1.96	3.94
C2H5N (Aziridine)	3.98	-0.02	-0.02	-0.01	0.93	4.00	3.97	3.63	2.35	4.33
C2H6 (Ethane)	3.37	-0.66	-0.59	-0.52	0.27	3.29	3.24	2.98	1.60	3.49
C2HF3 (Trifluoroethylene)	4.19	-0.59	-0.21	-0.09	0.98	4.30	4.20	3.75	2.49	4.77
C2N2 (Cyanogen)	5.48	-1.02	-1.14	-1.14	-0.01	4.88	4.47	3.72	2.58	6.06
C3H4 (Cyclopropene)	4.88	-1.04	-0.89	-0.66	0.56	4.27	4.17	3.62	2.21	4.23
C3H6 (Cyclopropane)	3.09	-0.03	-0.02	-0.02	0.85	3.74	3.72	3.46	1.58	4.01
C3H8 (Propane)	3.90	-0.01	-0.01	-0.03	0.85	3.83	3.81	3.50	2.18	3.96
C3O2 (Carbon suboxide)	4.10	-2.40	-1.99	-2.04	-0.57	3.97	3.63	3.01	1.76	4.59
C4H2 (Diacetylene)	3.42	-2.31	-1.81	-1.57	-0.51	2.82	2.80	2.72	1.48	3.05
C4H4O (Furan)	3.20	-1.21	-0.95	-0.79	0.34	3.77	3.68	3.16	1.60	3.20
C4H6 (Cyclobutene)	5.09	-0.65	-0.28	-0.17	0.80	3.57	3.59	3.35	2.00	3.67
C4N2 (2-Butynedinitrile)	3.22	-1.57	-1.72	-1.86	-1.14	2.84	2.54	2.00	0.73	3.75
CCl4 (Carbon tetrachloride)	5.03	-0.13	-1.09	-1.03	0.17	5.43	5.00	4.12	2.94	5.96
CF2Cl2 (Difluorodichloromethane)	5.89	-0.33	-0.30	-0.30	1.25	6.26	5.99	5.18	3.83	6.43
CF2O (Carbonic difluoride)	6.47	-1.52	-1.09	-1.01	0.62	5.18	5.05	4.46	2.94	5.53
CF3Br (Bromotrifluoromethane)	3.84	-0.41	-0.38	-0.11	1.32	6.58	3.90	3.30	1.85	4.33
CF3Cl (Methane, chlorotrifluoro-)	4.18	-0.44	-0.40	-0.38	1.44	4.45	4.37	5.32	2.38	4.65
CF4 (Carbon tetrafluoride)	4.30	-1.13	-1.01	-0.67	0.01	4.04	3.92	3.49	1.91	4.67
CFCl3 (Trichloromonofluoromethane)	5.53	-0.58	-0.56	-0.55	0.81	5.89	5.49	4.67	3.37	6.18
CH2CCH2 (Allene)	3.59	-0.80	-0.45	-0.37	0.84	3.81	3.81	3.51	2.13	3.92
CH2CCl2 (Ethene, 1,1-dichloro-)	4.15	-1.26	-1.18	-0.73	0.23	4.45	4.36	3.85	2.29	4.06

CH2CF2 (Ethene, 1,1-difluoro-)	4.32	-0.72	-0.29	-0.13	0.90	4.00	3.96	3.63	2.29	4.21
CH2CHCHO (Acrolein)	6.68	-0.21	-0.18	-0.06	1.59	6.87	6.48	5.62	4.69	8.23
CH2CHCl (Ethene, chloro-)	4.00	-1.14	-1.03	-0.98	0.38	4.17	4.07	3.56	2.13	3.92
CH2CHF (Ethene, fluoro-)	4.03	-1.13	-0.70	-0.59	0.75	3.83	3.82	3.54	2.19	4.04
CH2Cl2 (Methylene chloride)	4.95	-0.19	-0.16	-0.14	1.21	5.20	5.07	4.51	3.10	5.30
CH2CO (Ketene)	4.08	-1.99	-1.59	-1.49	0.05	4.14	4.11	3.74	2.38	4.39
CH2F2 (Methane, difluoro-)	4.53	0.00	0.00	-0.03	0.96	4.14	4.06	3.73	2.49	4.67
CH3 (Methyl radical)	4.04	-3.34	-2.43	-1.95	-0.92	4.10	3.73	3.13	1.27	1.61
CH3CCCH3 (2-Butyne)	3.57	0.01	0.00	-0.01	0.81	3.70	3.70	3.42	2.07	3.84
CH3CCH (Propyne)	3.52	0.01	0.00	-0.01	0.81	4.34	4.17	3.54	2.08	3.88
CH3CH2Cl (Ethyl chloride)	4.09	-0.15	-0.06	-0.04	0.86	4.39	4.26	3.70	2.40	4.64
CH3CH2OH (Ethanol)	4.45	-0.03	-0.02	0.00	1.05	4.46	4.39	3.95	2.69	5.07
CH3Cl (Methyl chloride)	4.46	-0.22	-0.14	-0.11	0.98	4.60	4.47	3.92	2.63	4.90
CH3COCl (Acetyl Chloride)	4.78	-0.21	-0.18	-0.06	0.31	4.80	4.88	4.50	3.04	4.86
CH3F (Methyl fluoride)	4.44	0.00	-0.01	-0.02	0.92	4.22	4.10	3.71	2.44	4.78
CH3NHCH3 (Dimethylamine)	3.87	-0.01	-0.01	-0.03	0.90	3.97	3.96	3.61	2.30	4.29
CH3NO2 (Methane, nitro-)	6.94	-0.25	-0.21	-0.11	-0.73	5.13	4.65	3.60	2.96	6.02
CH3OCH3 (Dimethyl ether)	3.81	0.01	0.00	-0.03	0.85	3.87	3.85	3.51	2.17	4.08
CH3OH (Methyl alcohol)	4.67	-0.03	-0.03	0.00	1.09	4.57	4.48	4.02	2.78	5.23
CH3SH (Methanethiol)	4.33	-0.07	-0.05	-0.03	1.01	4.62	4.50	3.98	2.58	4.67
CH3SiH3 (Methyl silane)	3.78	-0.07	-0.12	-0.06	0.84	3.93	3.91	3.58	2.26	4.12
CH4 (Methane)	4.34	-0.05	-0.06	-0.07	0.91	4.24	4.17	3.81	2.43	4.53
CHCl3 (Chloroform)	4.99	-0.68	-0.67	-0.65	0.68	5.28	5.11	4.46	3.08	5.45
CHF3 (Methane, trifluoro-)	4.44	-0.10	-0.09	-0.08	0.88	4.12	4.03	3.69	2.43	4.65
CHONH2 (Formamide)	4.93	-0.23	-0.09	-0.09	1.23	5.28	5.15	4.48	3.55	6.31
Cl (Chlorine atom)	-0.11	-8.27	-8.10	-8.72	-6.17	-0.74	-1.27	-2.22	-3.06	1.98
Cl2 (Chlorine diatomic)	7.05	-0.42	-0.38	-0.33	1.46	7.01	6.54	5.61	4.48	8.34
ClF (Chlorine monofluoride)	8.09	-4.46	-4.34	-0.34	-2.43	7.68	2.73	1.80	5.20	9.66
ClF3 (Chlorine trifluoride)	7.48	-0.42	-0.38	-0.33	1.53	7.25	6.78	5.80	4.85	9.61
ClO (Monochlorine monoxide)	4.07	-4.22	-4.14	-4.25	-1.93	3.93	3.39	2.27	1.36	6.30
CO (Carbon monoxide)	6.87	-1.31	-1.21	-0.94	1.00	6.73	6.35	5.36	4.29	7.60
CO2 (Carbon dioxide)	3.34	-2.03	-1.78	-1.24	-0.65	3.41	3.28	2.95	1.23	3.46
CS (Carbon monosulfide)	6.47	-0.76	-0.71	-0.54	1.30	7.00	6.51	5.54	4.47	8.83
CS2 (Carbon disulfide)	3.35	-2.60	-2.47	-3.06	-1.13	6.61	6.19	5.39	0.15	2.97
F (Fluorine atom)	0.40	- 12.20	- 10.98	-10.32	-7.86	-1.57	-2.15	-3.40	-3.10	3.48
F2 (Fluorine diatomic)	10.99	-0.70	-0.60	-0.18	2.65	8.83	8.48	7.37	7.88	5.15
F2O (Difluorine monoxide)	6.50	-3.74	-3.62	-3.30	-0.76	5.35	4.92	3.82	3.74	10.11

FCN (Cyanogen fluoride)	5.83	-0.26	-0.21	-0.06	1.27	5.85	5.65	4.95	3.42	6.25
H (Hydrogen atom)	2.01	-4.13	-2.73	-97.60	-1.12	0.39	0.26	-0.24	-15.16	-50.86
H2CO (Formaldehyde)	4.16	-2.70	-2.24	-2.05	-0.57	3.93	3.89	3.32	1.99	4.31
H2CS (Thioformaldehyde)	3.05	-3.49	-3.12	-3.19	-1.69	2.99	2.50	1.92	0.57	3.87
H2O (Water)	5.54	-0.09	-0.09	0.00	1.22	5.25	5.14	4.55	3.25	6.12
H2O2 (Hydrogen peroxide)	6.95	-0.55	-0.45	-0.16	1.95	6.45	6.32	5.58	4.76	8.71
H2S (Hydrogen sulfide)	4.50	-0.09	-0.09	-0.07	0.99	4.49	4.45	4.02	2.54	4.57
HCCCN (Cyanoacetylene)	3.58	-1.71	-1.83	-1.92	-0.75	3.63	3.41	2.85	1.54	3.92
HCCF (Fluoroacetylene)	4.36	-0.16	-0.12	-0.04	1.02	4.45	4.37	3.92	2.59	4.84
HCl (Hydrogen sulfide)	5.26	-0.19	-0.16	-0.12	1.18	5.15	5.02	4.45	3.10	5.54
HCN (Hydrogen cyanide)	4.86	-0.77	-0.79	-0.50	0.76	4.51	4.35	3.75	2.70	5.07
HCO (Formyl radical)	7.51	-0.77	-0.53	-0.52	1.48	7.27	6.78	5.78	4.61	7.82
HCOOH (Formic acid)	6.15	-0.26	-0.22	-0.07	1.93	6.28	6.16	5.49	4.62	8.00
He (Helium atom)	3.16	-4.62	-5.03	-5.86	-3.40	1.61	1.35	0.15	-1.20	1.89
HF (Hydrogen fluoride)	6.27	-0.10	-0.10	0.04	1.37	5.60	5.45	4.80	3.67	7.04
Li (Lithium atom)	2.89	-0.57	-0.11	0.14	0.15	3.64	3.70	3.58	1.96	-21.00
Mg (Magnesium atom)	3.48	-0.87	-0.81	-0.50	0.15	3.48	3.47	3.13	1.49	2.80
N (Nitrogen atom)	4.29	-5.20	-4.59	-4.57	-2.78	3.40	2.91	1.93	-0.01	1.33
N2 (Nitrogen diatomic)	4.78	-3.51	-2.95	-2.67	-1.17	4.23	3.79	3.07	1.84	5.17
N2H4 (Hydrazine)	4.68	-0.01	-0.01	-0.03	1.05	4.52	4.48	4.05	2.63	4.83
N2O (Nitrous oxide)	6.14	-1.50	-1.13	-2.11	-0.80	4.06	3.92	3.23	1.74	5.91
Na (Sodium atom)	2.12	-1.16	-0.09	0.49	-0.46	3.23	3.28	3.18	1.45	-16.01
NaCl (Sodium Chloride)	3.51	-0.02	-0.02	-0.04	0.83	3.63	3.63	3.43	2.09	4.03
Ne (Neon atom)	8.66	-0.10	-0.18	0.29	1.67	7.75	7.30	6.22	4.87	8.78
NF3 (Nitrogen trifluoride)	6.55	-0.37	-0.33	-0.17	1.80	6.73	6.56	5.76	4.19	7.69
NH (Imidogen)	9.56	-0.60	-0.38	0.40	2.18	8.59	8.07	6.96	6.17	9.92
NH2 (Amino radical)	9.30	-0.02	0.32	1.01	2.84	9.15	8.56	7.43	6.67	10.96
NH3 (Ammonia)	4.77	-0.05	-0.07	-0.04	1.05	4.70	4.63	4.16	2.72	4.99
NO (Nitric oxide)	3.97	-4.75	-4.57	-4.28	-2.63	3.00	2.45	1.55	0.55	5.49
NO2 (Nitrogen dioxide)	7.14	-1.75	-1.53	-1.27	0.87	6.75	6.29	5.27	4.50	9.72
O (Oxygen atom)	2.23	-8.72	-7.86	-7.12	-5.22	0.86	0.37	-0.68	-1.07	4.20
O2 (Oxygen diatomic)	3.91	-6.10	-5.33	-4.73	-3.24	2.97	2.46	1.31	0.84	6.65
O3 (Ozone)	5.71	-3.55	-3.42	-3.17	-0.94	5.15	4.62	3.50	2.70	6.85
OCS (Carbonyl sulfide)	4.53	-1.67	-1.37	-1.58	0.12	4.69	4.53	3.85	2.56	4.83
OH (Hydroxyl radical)	7.24	-3.69	-3.36	-2.66	-0.24	6.29	5.75	4.54	4.58	11.03
P (Phosphorus atom)	2.74	-4.08	-3.51	-4.14	-2.44	2.41	1.99	1.41	-0.87	-0.39
P2 (Phosphorus diatomic)	3.32	-2.45	-2.38	-2.25	-1.04	3.84	3.47	2.74	1.08	3.75
PF3 (Phosphorus trifluoride)	4.87	-0.96	-0.78	-0.55	0.63	5.02	4.86	4.20	2.64	5.02

PH3 (Phosphine)	4.09	-0.05	-0.05	-0.03	0.88	4.12	4.11	3.76	2.26	4.09
S (Sulfur atom)	1.26	-6.51	-5.94	-6.35	-4.25	0.70	0.29	-0.43	-1.27	3.05
S2 (Sulfur diatomic)	3.32	-3.46	-3.20	-3.08	-1.74	3.95	3.33	2.33	0.66	4.04
Si (Silicon atom)	1.76	-4.12	-4.05	-4.41	-2.66	2.00	1.66	1.08	-0.73	-0.67
Si2H6 (Disilane)	3.60	-0.44	-0.40	-0.30	0.45	4.02	3.93	3.40	1.84	3.57
SiF2 (Silicon difluoride)	5.37	-1.26	-1.20	-1.07	0.26	5.44	5.07	4.28	2.64	5.51
SiF4 (Silicon tetrafluoride)	4.45	-1.19	-1.14	-0.96	0.03	4.23	4.10	3.51	2.04	4.95
SiH3 (Silyl)	2.59	-3.29	-2.95	-3.05	-1.81	2.73	2.41	1.78	-0.51	-0.60
SiH4 (Silane)	3.96	-0.07	-0.07	-0.06	0.82	4.00	3.96	3.63	2.17	4.16
SiO (Silicon monoxide)	5.88	-0.63	-0.58	-0.46	0.95	5.91	5.61	4.88	3.38	6.27
SO2 (Sulfur dioxide)	7.27	-0.56	-0.51	-0.39	1.45	7.06	6.63	5.68	4.65	9.16
MAE		6.16	5.98	6.62	4.56	0.48	0.59	1.11	2.44	1.69
MSE		-6.16	-5.98	-6.62	-4.56	-0.13	-0.41	-1.03	-2.44	-0.48
RMS		6.48	6.28	10.91	4.80	0.74	0.96	1.46	2.86	5.69

Table S13. Statistical errors (in eV) of CCSD and CCSD(T) methods for IP(1) (with respect to the experimental data).

Property	Error	CCSD	CCSD(T)
IP(1)	MSE	0.06	0.07
(121)	MAE	0.17	0.14
	RMS	0.25	0.22

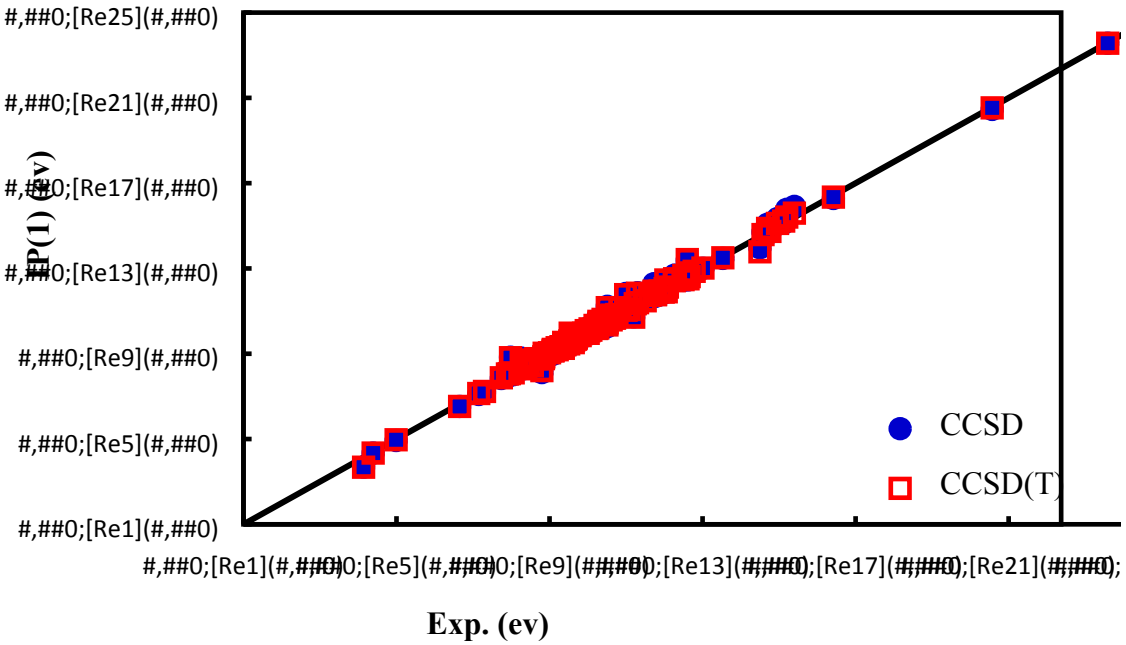

Figure 1. IP(1) calculated using CCSD and CCSD(T) methods with respect to the experimental data.

Table S14. Statistical errors (in eV) of CCSD for IP(1), EA(1), and Eg(1) (with respect to CCSD(T)).

Property	Error	CCSD
IP(1)	MSE	-0.01
	MAE	0.10
	RMS	0.12
EA(1)	MSE	-0.02
	MAE	0.04
	RMS	0.07
Eg(1)	MSE	0.01
	MAE	0.10
	RMS	0.13

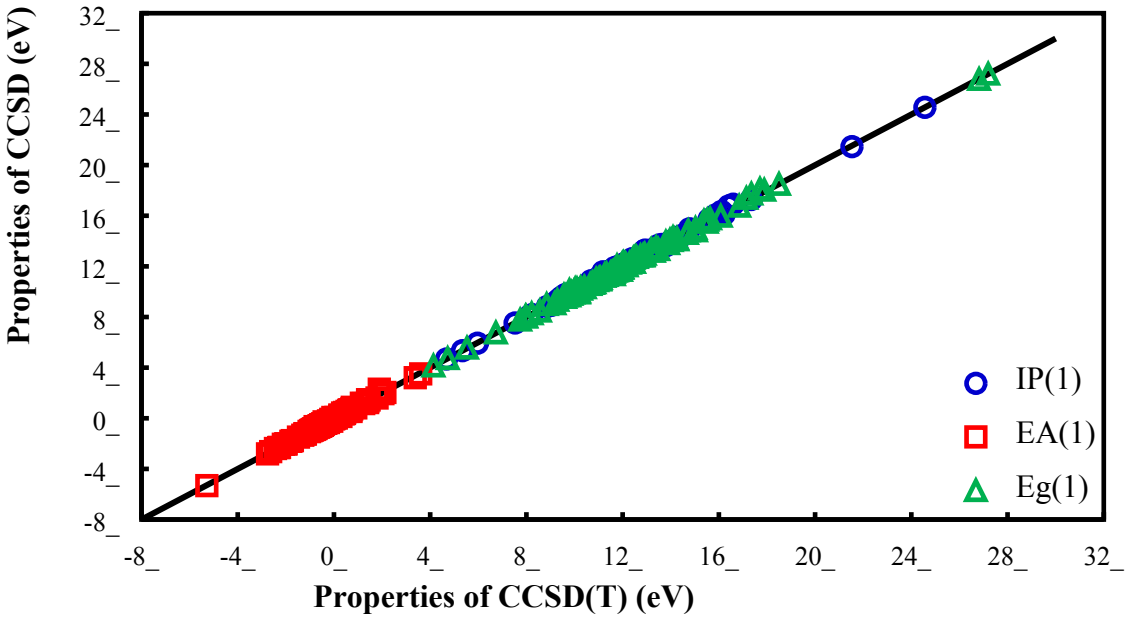

Figure 2. IP(1), EA(1), and Eg(1) calculated using CCSD with respect to those calculated using CCSD(T).

Table S15. Statistical errors (in eV) of 9 density functional methods for vertical ionization

potentials (with respect to the experimental data).

Property	Error	LDA	PBE	M06L	B3LYP	ωB97	ωB97X	ωB97X-D	M06-2X	M06-HF
IP(1)	MSE	0.45	-0.25	-0.30	-0.03	**-0.01**	**-0.01**	-0.03	0.09	0.41
	MAE	0.56	0.35	0.36	0.23	0.20	0.19	0.19	**0.18**	0.46
	RMS	0.63	0.51	0.48	0.33	0.28	0.27	**0.26**	0.27	0.60
IP(2)	MSE	-3.86	-4.44	-4.29	-3.19	**-0.28**	-0.53	-1.06	-1.51	0.89
	MAE	3.86	4.44	4.29	3.19	**0.42**	0.55	1.06	1.51	0.99
	RMS	3.98	4.55	4.39	3.27	**0.67**	0.80	1.24	1.59	1.15

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