Supplementary Information: On The Relation Between Equation-of-Motion Coupled-Cluster Theory and the GW Approximation

Formula	EOM-linCCSD	EOM-CC2	EOM-MBPT2	P-EOM-CC2	P-EOM-MBPT2
He	24.52	24.35	24.36	24.55	24.56
Ne	21.24	21.27	21.11	20.78	20.65
Ar	15.68	15.50	15.55	15.59	15.63
Kr	14.03	13.87	13.88	13.96	13.98
Xe	12.28	12.12	12.13	12.24	12.25
H_2	16.42	16.20	16.22	16.31	16.33
Li_2	5.37	4.97	4.98	5.17	5.18
Na_2	5.04	4.74	4.74	4.86	4.86
Na_4	4.44	4.03	4.05	4.11	4.13
Na_6	4.60	4.24	4.27	4.32	4.36
K_2	4.21	3.94	3.95	4.03	4.04
Rb_2	4.06	3.81	3.80	3.87	3.87
N_2	15.66	15.65	15.84	15.62	15.81
P_2	10.80	10.62	10.65	10.67	10.70
As_2	10.14	10.01	10.02	10.03	10.05
F_2	15.68	15.65	15.57	15.29	15.25
Cl_2	11.56	11.33	11.39	11.40	11.46
Br_2	10.63	10.43	10.46	10.49	10.53
I_2	9.63	9.62	9.70	9.57	9.66
CH_4	14.44	14.24	14.29	14.31	14.36
C_2H_6	12.78	12.57	12.62	12.64	12.69
C_3H_8	12.14	11.98	12.04	11.97	12.05
C_4H_{10}	11.66	11.51	11.61	11.48	11.58
C_2H_4	10.87	10.61	10.66	10.59	10.63
C_2H_2	11.69	11.58	11.66	11.52	11.58
C_4	11.51	11.32	11.38	11.35	11.41
C_3H_6	10.97	10.84	10.91	10.78	10.84
C_6H_6	9.56	9.47	9.54	9.40	9.46
C_8H_8	8.64	8.46	8.53	8.36	8.43
C_5H_6	8.94	8.75	8.81	8.68	8.72
C_2H_3F	10.78	10.55	10.61	10.48	10.54
C_2H_3Cl	10.30	10.06	10.13	10.07	10.13
C_2H_3Br	9.46	9.24	9.29	9.25	9.29
C_2H_3I	9.49	9.40	9.47	9.38	9.45
CF_4	16.31	16.35	16.29	15.94	15.93
CCl_4	11.70	11.49	11.58	11.56	11.64
CBr_4	10.56	10.38	10.44	10.45	10.51
CI_4	9.38	9.39	9.51	9.35	9.45
SiH_4	12.89	12.62	12.66	12.91	12.95
GeH_4	12.58	12.34	12.38	12.59	12.64
Si_2H_6	10.79	10.50	10.56	10.71	10.78
Si_5H_{12}	9.46	9.19	9.28	9.35	9.45
LiH	8.00	7.73	7.76	7.98	8.01
KH	6.21	5.90	5.90	6.09	6.10
BH_3	13.35	13.09	13.13	13.30	13.34
B_2H_6	12.34	12.09	12.15	12.31	12.38
NH_3	10.84	10.73	10.76	10.63	10.66
HN_3	10.95	*	11.06	*	10.92
PH_3	10.66	10.34	10.39	10.50	10.55
AsH_3	10.50	10.26	10.31	10.39	10.44
SH_2	10.43	10.19	10.24	10.30	10.35
FH	15.95	15.99	15.85	15.52	15.41
ClH	12.72	12.50	12.55	12.59	12.64
LiF	11.36	11.51	11.19	10.69	10.51
F_2Mg	13.79	13.93	13.64	13.11	12.96
TiF_4	15.75	16.01	15.80	14.95	15.06
AlF_3	15.37	15.47	15.29	14.84	14.75

BF	11.32	*	10.93	*	11.09
SF_4	12.85	12.73	12.75	12.49	12.55
BrK	8.25	8.08	8.07	8.09	8.09
GaCl	9.90	9.63	9.64	9.69	9.72
NaCl	9.21	9.03	9.04	8.98	9.00
$MgCl_2$	11.84	11.65	11.69	11.66	11.70
AlI_3	9.91	9.91	10.01	9.91	10.00
BN	11.84	*	12.09	*	11.69
NCH	14.01	*	14.07	*	13.95
PN	11.96	12.01	12.08	11.72	11.81
H_2NNH_2	9.71	9.60	9.61	9.51	9.53
H_2CO	10.92	*	10.77	*	10.50
CH_4O	11.04	10.99	10.94	10.76	10.73
C_2H_6O	10.70	10.65	10.60	10.41	10.38
C_2H_4O	10.35	10.28	10.20	9.98	9.93
$C_4H_{10}O$	9.86	9.83	9.76	9.55	9.51
CH_2O_2	11.57	11.59	11.48	11.21	11.15
HOOH	11.50	11.48	11.43	11.22	11.19
H_2O	12.54	12.53	12.47	12.21	12.18
CO_2	13.87	*	13.99	*	13.73
CS_2	10.21	*	10.14	*	10.18
OCS	11.40	*	11.38	*	11.38
OCSe	10.66	*	10.62	*	10.61
CO	14.45	*	14.58	*	14.67
O_3	13.20	*	13.22	*	12.64
SO_2	12.54	*	12.57	*	12.28
BeO	9.80	*	9.84	*	9.16
MgO	9.31	*	8.04	*	6.68
C_7H_8	9.15	9.08	9.14	8.99	9.05
C_8H_{10}	9.10	9.04	9.11	8.95	9.01
C_6F_6	10.38	10.28	10.46	10.15	10.32
C_6H_5OH	8.92	8.87	8.92	8.74	8.79
$C_6H_5NH_2$	8.19	8.13	8.19	8.02	8.08
C_5H_5N	9.89	9.84	9.90	9.58	9.65
$C_5H_5N_5O$	8.40	8.32	8.37	8.15	8.21
$C_5H_5N_5$	8.64	8.59	8.64	8.43	8.48
$C_4H_5N_3O$	9.07	9.00	9.03	8.81	8.84
$C_5H_6N_2O_2$	9.34	9.29	9.43	9.16	9.29
$C_4H_4N_2O_2$	9.74	9.70	9.83	9.57	9.70
CH_4N_2O	10.23	10.26	10.15	9.88	9.82
Ag_2	7.62	7.63	7.47	7.54	7.42
Cu_2	7.56	7.59	7.22	7.41	7.17
NCCu	10.32	11.27	10.81	10.35	9.86

TABLE I: Full data set of first ionization potentials predicted by approximations to EOM-CCSD, as summarized in the text. Asterisks indicate molecules for which ground state CC2 did not converge.

Formula	EOM-linCCSD	EOM-CC2	EOM-MBPT2	P-EOM-CC2	P-EOM-MBPT2
He	22.22	22.15	22.15	22.28	22.27
Ne	20.84	20.83	20.90	20.92	20.99
Ar	14.74	14.71	14.69	14.77	14.75
Kr	10.42	10.39	10.39	10.45	10.44
Xe	7.73	7.71	7.71	7.76	7.76
H_2	4.23	4.17	4.15	4.25	4.24
Li_2	-0.08	-0.21	-0.22	-0.09	-0.10
Na_2	-0.20	-0.36	-0.37	-0.27	-0.29
Na_4	-0.01	-0.01	-0.04	-0.13	-0.15
Na_6	-0.20	-0.15	-0.20	-0.12	-0.16
K_2	-0.24	-0.43	-0.43	-0.37	-0.40
Rb_2	-0.28	-0.61	-0.47	-0.40	-0.43
N_2	3.18	3.09	2.98	3.28	3.12
P_2	0.10	-0.26	-0.25	-0.10	-0.22

As_2	-0.03	-0.26	-0.33	-0.24	-0.34
F_2	0.76	0.33	0.44	0.46	0.56
Cl_2	-0.05	-0.37	-0.40	-0.30	-0.34
Br_2	-0.81	-1.09	-1.10	-1.01	-1.03
I_2	-1.37	-1.49	-1.56	-1.51	-1.59
CH_4	3.46	3.42	3.41	3.49	3.49
C_2H_6	3.12	3.08	3.08	3.15	3.14
C_3H_8	2.96	2.92	2.91	2.98	2.98
C_4H_{10}	2.90	2.85	2.85	2.91	2.91
C_2H_4	2.76	2.53	2.46	2.61	2.54
C_2H_2	3.59	3.45	3.39	3.58	3.47
C_4	-2.18	-2.43	-0.03	-2.45	-0.06
C_3H_6	3.47	3.42	3.42	3.48	3.48
C_6H_6	1.98	1.85	1.76	1.78	1.70
C_8H_8	1.01	0.77	0.69	0.68	0.62
C_5H_6	1.97	1.74	1.67	1.71	1.65
C_2H_3F	2.95	2.74	2.63	2.79	2.70
C_2H_3Cl	2.28	2.05	1.95	2.05	1.97
C_2H_3Br	2.18	1.97	1.88	1.96	1.89
C_2H_3I	1.48	1.42	1.36	1.38	1.32
CF_4	4.90	4.88	4.91	4.92	4.95
CCl_4	0.96	0.83	0.72	0.70	0.62
CBr_4	-0.39	-0.48	-0.58	-0.63	-0.70
CI_4	-1.51	-1.46	-1.60	-1.69	-1.79
SiH_4	3.12	3.03	3.01	3.15	3.14
GeH_4	3.18	3.09	3.09	3.21	3.21
Si_2H_6	2.29	2.16	2.13	2.29	2.26
Si_5H_{12}	0.85	0.68	0.66	0.76	0.75
LiH	0.10	0.06	0.06	0.11	0.10
KH	-0.02	-0.06	-0.07	-0.03	-0.04
BH_3	0.35	0.24	0.21	0.42	0.39
B_2H_6	1.24	1.11	1.08	1.23	1.20
NH_3	2.85	2.81	2.82	2.87	2.87
HN_3	2.27	*	2.01	*	1.93
PH_3	2.97	2.89	2.88	2.98	2.97
AsH_3	2.88	2.81	2.79	2.88	2.87
SH_2	2.81	2.72	2.71	2.80	2.78
FH	3.08	3.07	3.08	3.11	3.12
ClH	2.73	2.62	2.60	2.69	2.67
LiF	-0.02	-0.02	-0.03	-0.01	-0.02
F_2Mg	-0.02	-0.01	-0.02	0.02	0.02
TiF_4	-0.53	0.01	-0.44	-0.07	-0.95
AlF_3	0.69	0.69	0.69	0.74	0.75
BF	1.59	*	1.35	*	1.54
SF_4	1.09	0.99	0.80	0.94	0.79
BrK	-0.44	-0.45	-0.46	-0.42	-0.43
GaCl	0.34	0.16	0.13	0.24	0.19
NaCl	-0.58	-0.59	-0.60	-0.57	-0.58
$MgCl_2$	-0.16	-0.21	-0.24	-0.17	-0.19
AlI_3	-0.21	-0.23	-0.33	-0.32	-0.41
BN	-3.97	*	-3.57	*	-3.63
NCH	3.32	*	3.14	3.39	3.24
PN	0.67	0.06	0.45	0.69	0.48
H_2NNH_2	2.52	2.49	2.49	2.53	2.54
H_2CO	1.81	*	1.61	*	1.71
CH_4O	3.04	3.00	3.01	3.06	3.07
C_2H_6O	2.87	2.84	2.85	2.89	2.91
C_2H_4O	2.06	1.93	1.87	1.97	1.92
$C_4H_{10}O$	2.98	2.94	2.94	3.00	3.00
CH_2O_2	2.85	2.81	2.69	2.84	2.74
HOOH	3.04	3.00	3.02	3.03	3.06
H_2O	2.89	2.87	2.88	2.92	2.93
CO_2	2.83	*	2.76	*	2.78
CS_2	0.54	*	0.20	*	0.10

OCS	2.05	*	1.80	*	1.74
OCSe	1.66	*	1.41	*	1.29
CO	1.42	*	1.10	*	1.23
O_3	0.09	*	-1.16	*	-1.23
SO_2	-0.04	*	-0.33	*	-0.31
BeO	-2.22	*	-2.11	*	-2.09
MgO	-1.13	*	-1.11	*	-1.16
C_7H_8	1.91	1.79	1.71	1.71	1.64
C_8H_{10}	1.95	1.84	1.76	1.75	1.68
C_6F_6	1.27	1.23	1.02	1.06	0.88
C_6H_5OH	1.83	1.71	1.61	1.63	1.54
$C_6H_5NH_2$	2.03	1.91	1.82	1.83	1.75
C_5H_5N	1.46	1.35	1.26	1.27	1.20
$C_5H_5N_5O$	*	1.75	1.59	1.59	1.44
$C_5H_5N_5$	1.55	1.46	1.36	1.30	1.22
$C_4H_5N_3O$	1.29	1.08	0.85	0.94	0.76
$C_5H_6N_2O_2$	1.03	0.92	0.71	0.78	0.61
$C_4H_4N_2O_2$	0.97	0.83	0.61	0.72	0.54
CH_4N_2O	2.35	2.32	2.30	2.36	2.35
Ag_2	-0.63	-0.70	-0.70	-0.72	-0.72
Cu_2	-0.27	-0.39	-0.33	-0.37	-0.29
NCCu	-1.11	-0.97	-0.93	-0.93	-0.87

TABLE II: Full data set of first electron affinities predicted by approximations to EOM-CCSD, as summarized in the text. Asterisks indicate molecules for which ground state CC2 did not converge.