The GW Method for Quantum Chemistry applications: Theory and Implementation

Supporting Information

M.J. van Setten,[*,†] F. Weigend,[†,‡] and F. Evers[†,¶]

Institute of Nanotechnology, Karlsruhe Institute of Technology, P.O.Box 3640 D-76021 Karlsruhe, Germany, Institute of Physical Chemistry, Karlsruhe Institute of Technology, P.O.Box 3640 D-76021 Karlsruhe, Germany, and Institute of Theoretical Condensed Matter, Karlsruhe Institute of Technology, P.O.Box 3640 D-76021 Karlsruhe, Germany

E-mail: michiel.setten@kit.edu

[*]To whom correspondence should be addressed

[†]Institute of Nanotechnology, Karlsruhe Institute of Technology, P.O.Box 3640 D-76021 Karlsruhe, Germany

[‡]Institute of Physical Chemistry, Karlsruhe Institute of Technology, P.O.Box 3640 D-76021 Karlsruhe, Germany

[¶]Institute of Theoretical Condensed Matter, Karlsruhe Institute of Technology, P.O.Box 3640 D-76021 Karlsruhe, Germany

1 Ionization Potentials

Table 1: Experimental I_P, minus DFT PBE HOMO energy, and minus G_0W_0@PBE HOMO energies of the GW27 molecules.

	exp IP	PBE	G_0W_0@PBE
H_2	15.42	10.245	15.726
Li_2	5.11	3.213	4.905
Na_2	4.89	3.125	4.74
Cs_2	3.70	2.3	3.35
F_2	15.70	8.97	14.441
N_2	15.58	10.197	14.514
BF	11.00	6.795	10.504
LiH	7.90	4.363	6.644
CO_2	13.78	9.02	12.791
H_2O	12.62	7.019	11.761
NH_3	10.85	6.017	10.103
SiH_4	12.30	8.472	12.227
SF_4	12.30	8.094	11.793
Au_2	9.50	6.324	8.754
Au_4	8.60	5.632	7.346
Methane	13.60	9.441	13.84
Ethane	12.00	8.127	12.268
Propane	11.51	7.665	11.602
Butane	11.09	7.579	11.156
Isobutane	11.13	7.599	11.185
Ethylene	10.68	6.775	10.218
Acetone	9.70	5.586	8.584
Acrolein	10.11	5.956	8.914
Benzene	9.24	6.394	8.653
Naphthalene	8.09	5.497	7.493
Anthracene	7.40	4.964	6.651
Naphthacene	6.97	4.648	6.115

2 Electron Affinities

Table 2: Experimental E_A, minus DFT PBE LUMO energy, and minus G_0W_0@PBE LUMO energies of the GW27 molecules with positive E_A.

	exp IP	PBE	G_0W_0@PBE
Na_2	0.43	1.806	0.316
Cs_2	0.469	1.517	0.38
LiH	0.342	1.571	-0.278
Au_2	1.951	4.275	1.619
Au_4	2.66	4.675	2.385
Naphthalene	-0.2	2.005	0.655
Anthacene	0.53	2.681	0.325
Naphacene	1.067	3.054	0.869

3 Atomic structures

Table 3: Atomic structure of the GW27 molecules in xyz format

2			
H2			
H	-0.3836975	0.0000000	0.0000000
H	0.3836975	0.0000000	0.0000000
2			
Li2			
Li	-1.3977099	0.0000000	-0.0000000
Li	1.3977099	0.0000000	-0.0000000
2			
Na2			
Na	-1.5740776	0.0000000	0.0000000
Na	1.5740776	0.0000000	0.0000000
2			
Cs2			
Cs	0.0000000	0.0000000	-2.3617650
Cs	0.0000000	0.0000000	2.3617650
2			
F2			
F	0.0000000	0.0000000	-0.6670322
F	0.0000000	0.0000000	0.6670322
2			
N2			
N	0.0000000	0.0000000	-0.5559659
N	0.0000000	0.0000000	0.5559659
2			
BF			
B	0.0000000	0.0000000	-0.8139728
F	0.0000000	0.0000000	0.4631895
2			
LiH			
Li	-0.5434056	-0.0000000	0.0000000
H	1.0729606	0.0000000	0.0000000

3			
CO2			
C	0.0000000	0.0000000	0.0000000
O	0.5291771	1.0486261	0.0000000
O	-0.5291771	-1.0486261	0.0000000
3			
H2O			
O	0.0000000	0.0000000	-0.0644484
H	0.7499149	0.0000000	0.5114912
H	-0.7499149	0.0000000	0.5114912
4			
NH3			
N	0.0000000	0.0000000	0.0683541
H	0.9293009	0.0000000	-0.3166152
H	-0.4646504	0.8047982	-0.3166152
H	-0.4646504	-0.8047982	-0.3166152
5			
SiH4			
Si	0.0529177	0.1058354	0.1587531
H	0.9220329	0.9749506	1.0278684
H	-0.8161975	0.9749506	-0.7103621
H	-0.8161975	-0.7632798	1.0278684
H	0.9220329	-0.7632798	-0.7103621
5			
SF4			
S	0.0000000	0.0000000	0.3863140
F	-1.6251188	0.0000000	0.2602782
F	1.6251188	0.0000000	0.2602782
F	0.0000000	1.1971807	-0.5862733
F	0.0000000	-1.1971807	-0.5862733
2			
Au2			
Au	0.0000000	0.0000000	-1.2651508
Au	0.0000000	0.0000000	1.2651508
4			
Au4			
Au	0.0000000	2.3977143	0.0000000
Au	-1.3405099	0.0000000	0.0000000
Au	1.3405099	0.0000000	0.0000000
Au	0.0000000	-2.3977143	0.0000000

5			
Methane			
C	0.0000000	0.0000000	0.0000000
H	0.6289005	0.6289005	0.6289005
H	-0.6289005	0.6289005	-0.6289005
H	-0.6289005	-0.6289005	0.6289005
H	0.6289005	-0.6289005	-0.6289005
8			
Ethane			
C	0.0000000	0.0000000	0.7612417
C	0.0000000	0.0000000	-0.7612417
H	-0.8801575	0.5081592	1.1576293
H	0.0000000	-1.0163184	1.1576293
H	0.8801575	0.5081592	1.1576293
H	0.0000000	1.0163184	-1.1576293
H	0.8801575	-0.5081592	-1.1576293
H	-0.8801575	-0.5081592	-1.1576293
11			
Propane			
C	-1.2815905	0.2673331	0.0000000
H	-2.1909375	-0.3681015	0.0000000
H	-1.3349663	0.9244301	0.8940038
H	-1.3349663	0.9244301	-0.8940038
C	0.0000085	-0.5738626	0.0000000
H	-0.0000333	-1.2472599	-0.8856770
H	-0.0000333	-1.2472599	0.8856770
C	1.2816026	0.2673234	0.0000000
H	1.3347951	0.9244017	0.8940310
H	1.3347951	0.9244017	-0.8940310
H	2.1911005	-0.3678557	0.0000000
14			
Butane			
C	-1.9527152	0.1314894	0.0000000
H	-2.7393561	-0.6239229	0.0000000
H	-2.0973811	0.7598934	0.8808897
H	-2.0973811	0.7598934	-0.8808897
C	-0.5693960	-0.5081130	0.0000000
H	-0.4705419	-1.1587500	-0.8735105
H	-0.4705419	-1.1587500	0.8735105
C	0.5693960	0.5081130	0.0000000
H	0.4705419	1.1587500	0.8735105
H	0.4705419	1.1587500	-0.8735105
C	1.9527152	-0.1314894	0.0000000
H	2.0973811	-0.7598934	0.8808897
H	2.7393561	0.6239229	0.0000000
H	2.0973811	-0.7598934	-0.8808897

14			
Isobutane			
C	0.0000000	0.0000000	-0.3626375
H	0.0000000	0.0000000	-1.4591256
C	0.7321192	-1.2680677	0.1046743
H	0.2324364	-2.1717001	-0.2598833
H	0.7627195	-1.3210689	1.1992425
H	1.7645292	-1.2871459	-0.2598833
C	0.7321192	1.2680677	0.1046743
C	-1.4642385	0.0000000	0.1046743
H	1.7645292	1.2871459	-0.2598833
H	-1.9969656	0.8845542	-0.2598833
H	0.7627195	1.3210689	1.1992425
H	-1.5254390	0.0000000	1.1992425
H	0.2324364	2.1717001	-0.2598833
H	-1.9969656	-0.8845542	-0.2598833
6			
Ethylene			
C	0.0000000	0.0000000	0.6608153
C	0.0000000	0.0000000	-0.6608153
H	0.9228996	0.0000000	1.2316760
H	-0.9228996	0.0000000	1.2316760
H	0.9228996	0.0000000	-1.2316760
H	-0.9228996	0.0000000	-1.2316760
10			
Acetone			
O	0.0229665	-1.2875087	0.0000000
C	1.2715587	0.7042968	0.0000000
C	-1.2957929	0.6663114	0.0000000
C	-0.0042867	-0.0967823	0.0000000
H	1.1060896	1.7732098	0.0000000
H	-2.1314185	-0.0154317	0.0000000
H	1.8602967	0.4419472	0.8699131
H	1.8602967	0.4419472	-0.8699131
H	-1.3599749	1.3078397	0.8731087
H	-1.3599749	1.3078397	-0.8731087
8			
Acrolein			
C	0.0000000	0.0000000	0.0000000
C	0.0000000	0.0000000	1.3399980
C	1.2557372	0.0000000	2.0650023
O	1.7840146	1.0565496	2.3699988
H	-0.9353046	0.0000000	-0.5399987
H	0.9353046	0.0000000	-0.5399987
H	-0.9353046	0.0000000	1.8800020
H	1.7233921	-0.9353046	2.3349991

12			
Benzene			
C	1.3892220	0.0000000	0.0000000
C	0.6946110	1.2031015	0.0000000
C	-0.6946110	1.2031015	0.0000000
C	-1.3892220	0.0000000	0.0000000
C	-0.6946110	-1.2031015	0.0000000
C	0.6946110	-1.2031015	0.0000000
H	2.4672443	0.0000000	0.0000000
H	1.2336222	2.1366963	0.0000000
H	-1.2336222	2.1366963	0.0000000
H	-2.4672443	0.0000000	0.0000000
H	-1.2336222	-2.1366963	0.0000000
H	1.2336222	-2.1366963	0.0000000
18			
Naphthalene			
C	-1.2485059	1.4004909	0.0000000
C	-2.4321204	0.7109279	0.0000000
C	-2.4321204	-0.7109279	0.0000000
C	-1.2485059	-1.4004909	0.0000000
C	0.0000000	-0.7097052	0.0000000
C	0.0000000	0.7097052	0.0000000
H	-1.2450605	2.4830537	0.0000000
H	-3.3730175	1.2448992	0.0000000
H	-3.3730175	-1.2448992	0.0000000
H	-1.2450605	-2.4830537	0.0000000
C	1.2485059	-1.4004909	0.0000000
C	1.2485059	1.4004909	0.0000000
C	2.4321204	-0.7109279	0.0000000
C	2.4321204	0.7109279	0.0000000
H	1.2450605	-2.4830537	0.0000000
H	1.2450605	2.4830537	0.0000000
H	3.3730175	-1.2448992	0.0000000
H	3.3730175	1.2448992	0.0000000

24			
Antracene			
C	-2.4927437	1.4151026	0.0000000
C	-3.6849291	0.7153027	0.0000000
C	-3.6849291	-0.7153027	0.0000000
C	-2.4927437	-1.4151026	0.0000000
C	-1.2327018	-0.7279406	0.0000000
C	-1.2327018	0.7279406	0.0000000
H	-2.4915355	2.5165432	0.0000000
H	-4.6429169	1.2575675	0.0000000
H	-4.6429169	-1.2575675	0.0000000
H	-2.4915355	-2.5165432	0.0000000
C	0.0000000	-1.4127552	0.0000000
C	0.0000000	1.4127552	0.0000000
C	1.2327018	-0.7279406	0.0000000
C	1.2327018	0.7279406	0.0000000
H	0.0000000	-2.5149158	0.0000000
H	0.0000000	2.5149158	0.0000000
C	2.4927437	-1.4151026	0.0000000
C	2.4927437	1.4151026	0.0000000
H	2.4915355	-2.5165432	0.0000000
H	2.4915355	2.5165432	0.0000000
C	3.6849291	-0.7153027	0.0000000
C	3.6849291	0.7153027	0.0000000
H	4.6429169	-1.2575675	0.0000000
H	4.6429169	1.2575675	0.0000000

30			
Naphthacene			
C	-3.7321288	1.4166040	0.0000000
C	-4.9214673	0.7163523	0.0000000
C	-4.9209221	-0.7177123	0.0000000
C	-3.7311047	-1.4170460	0.0000000
C	-2.4676344	-0.7303946	0.0000000
C	-2.4680387	0.7308193	0.0000000
H	-3.7317315	2.5180365	0.0000000
H	-5.8803104	1.2571074	0.0000000
H	-5.8793431	-1.2592179	0.0000000
H	-3.7298667	-2.5184317	0.0000000
C	-1.2417998	-1.4148941	0.0000000
C	-1.2421482	1.4158254	0.0000000
C	-0.0000513	-0.7308406	0.0000000
C	0.0000139	0.7319581	0.0000000
H	-1.2421126	-2.5168765	0.0000000
H	-1.2427819	2.5178834	0.0000000
C	2.4676541	-0.7304211	0.0000000
C	2.4679173	0.7308013	0.0000000
C	1.2417685	-1.4149873	0.0000000
C	1.2421702	1.4158665	0.0000000
H	1.2420119	-2.5169637	0.0000000
H	1.2428012	2.5178997	0.0000000
C	3.7312785	-1.4170211	0.0000000
C	3.7320472	1.4165786	0.0000000
H	3.7297314	-2.5184167	0.0000000
H	3.7316515	2.5180226	0.0000000
C	4.9210550	-0.7176896	0.0000000
C	4.9214072	0.7164320	0.0000000
H	5.8795553	-1.2590280	0.0000000
H	5.8801980	1.2572359	0.0000000