Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental information for: Local self-interaction correction method with a simple scaling factor

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Table S1 Comparison of non-self-consistent and fully self-consistent calculations for OSIC(w). MAEs of atoms $Z = 1 - 18$, AE6, and BH6 sets are shown.

Method	Atoms (E_h)	AE6 (kcal/mol)	BH6 (kcal/mol)
OSIC($w, k = 1$)			
non-SCF	0.074	33.7	3.58
SCF	0.075	33.6	3.65
OSIC($w, k = 2$)			
non-SCF	0.070	24.1	4.12
SCF	0.069	23.9	4.25
OSIC($w, k = 3$)			
non-SCF	0.135	17.8	4.60
SCF	0.132	17.6	4.77
OSIC($w, k = 4$)			
non-SCF	0.184	13.1	5.12
SCF	0.181	12.8	5.33

Table S2 Total energies of atoms (in E_h) for PZSIC, LSIC(z), and LSIC(w) with varying values in k using LSDA.

Z	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Accu}$
		$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
1	-0.500	-0.500	-0.500	-0.500	-0.500	-0.500	-0.500
2	-2.920	-2.920	-2.920	-2.920	-2.920	-2.920	-2.904
3	-7.509	-7.501	-7.503	-7.500	-7.498	-7.496	-7.478
4	-14.707	-14.678	-14.687	-14.678	-14.671	-14.666	-14.667
5	-24.726	-24.670	-24.681	-24.660	-24.646	-24.635	-24.654
6	-37.955	-37.867	-37.869	-37.833	-37.809	-37.792	-37.845
7	-54.741	-54.615	-54.603	-54.550	-54.518	-54.495	-54.589
8	-75.285	-75.101	-75.085	-75.007	-74.959	-74.923	-75.067
9	-100.012	-99.768	-99.729	-99.621	-99.554	-99.507	-99.734
10	-129.281	-128.971	-128.906	-128.769	-128.687	-128.630	-128.938
11	-162.673	-162.273	-162.210	-162.045	-161.948	-161.881	-162.255
12	-200.548	-200.046	-199.993	-199.800	-199.688	-199.612	-200.053
13	-242.920	-242.323	-242.270	-242.047	-241.919	-241.832	-242.346
14	-290.010	-289.313	-289.260	-289.007	-288.864	-288.767	-289.359
15	-341.982	-341.185	-341.130	-340.847	-340.689	-340.583	-341.259
16	-398.929	-398.018	-397.968	-397.653	-397.477	-397.359	-398.110
17	-461.059	-460.032	-459.983	-459.634	-459.442	-459.314	-460.148
18	-528.539	-527.396	-527.344	-526.964	-526.756	-526.618	-527.540
19	-601.004	-599.732	-599.695	-599.284	-599.061	-598.914	
20	-678.752	-677.340	-677.321	-676.878	-676.639	-676.483	
21	-761.957	-760.388	-760.375	-759.891	-759.632	-759.463	
22	-850.866	-849.128	-849.127	-848.602	-848.322	-848.140	
23	-945.513	-943.637	-943.624	-943.070	-942.777	-942.588	
24	-1046.123	-1044.167	-1044.119	-1043.548	-1043.249	-1043.056	
25	-1152.838	-1150.693	-1150.653	-1150.042	-1149.727	-1149.525	
26	-1265.725	-1263.386	-1263.355	-1262.701	-1262.364	-1262.149	
27	-1385.019	-1382.468	-1382.458	-1381.756	-1381.396	-1381.165	
28	-1510.546	-1507.950	-1507.897	-1507.191	-1506.833	-1506.606	
29	-1642.968	-1640.180	-1640.085	-1639.344	-1638.975	-1638.743	
30	-1782.107	-1779.074	-1779.009	-1778.220	-1777.828	-1777.582	
31	-1927.727	-1924.467	-1924.428	-1923.589	-1923.174	-1922.915	
32	-2080.027	-2076.542	-2076.527	-2075.642	-2075.205	-2074.933	
33	-2239.101	-2235.395	-2235.403	-2234.473	-2234.015	-2233.731	
34	-2404.970	-2401.038	-2401.072	-2400.096	-2399.617	-2399.319	
35	-2577.773	-2573.616	-2573.671	-2572.650	-2572.150	-2571.841	
36	-2757.608	-2753.224	-2753.301	-2752.237	-2751.717	-2751.396	
MAE	0.381	0.041	0.061	0.196	0.277	0.332	

†Reference [1]

Table S3 Total energies of atoms (in E_h) for OSIC(w) with varying values in k using LSDA.

Z	OSIC(w)			$E^{\dagger}_{Accu}$
	$k=1$	$k=2$	$k=3$	
1	-0.500	-0.500	-0.500	-0.500
2	-2.920	-2.920	-2.920	-2.904
3	-7.506	-7.504	-7.503	-7.478
4	-14.696	-14.690	-14.686	-14.667
5	-24.700	-24.687	-24.677	-24.654
6	-37.902	-37.876	-37.858	-37.845
7	-54.651	-54.611	-54.585	-54.589
8	-75.155	-75.095	-75.056	-75.067
9	-99.821	-99.736	-99.681	-99.734
10	-129.023	-128.912	-128.842	-128.938
11	-162.346	-162.208	-162.124	-162.255
12	-200.151	-199.987	-199.888	-200.053
13	-242.451	-242.260	-242.146	-242.346
14	-289.464	-289.245	-289.115	-289.359
15	-341.358	-341.111	-340.964	-341.259
16	-398.223	-397.945	-397.782	-398.110
17	-460.264	-459.954	-459.774	-460.148
18	-527.652	-527.310	-527.112	-527.540
19	-600.028	-599.656	-599.442	
20	-677.684	-677.280	-677.049	
21	-760.782	-760.339	-760.085	
22	-849.576	-849.092	-848.815	
23	-944.113	-943.596	-943.303	
24	-1044.646	-1044.106	-1043.801	
25	-1151.220	-1150.639	-1150.313	
26	-1263.976	-1263.350	-1262.998	
27	-1383.129	-1382.455	-1382.077	
28	-1508.602	-1507.919	-1507.539	
29	-1640.861	-1640.134	-1639.734	
30	-1779.822	-1779.042	-1778.615	
31	-1925.275	-1924.445	-1923.993	
32	-2077.411	-2076.534	-2076.057	
33	-2236.324	-2235.399	-2234.899	
34	-2402.033	-2401.061	-2400.536	
35	-2574.673	-2573.654	-2573.106	
36	-2754.345	-2753.279	-2752.706	
MAE	0.074	0.070	0.135	

†Reference [1]

Table S4 Δ-SCF ionization potentials (in eV) for PZSIC, LSIC(z), and LSIC(w,k) where $k = 1-4$ with LSDA.

Z	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Exp}$
		$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
2	25.032	25.032	25.032	25.032	25.032	25.032	24.587
3	5.539	5.307	5.373	5.292	5.237	5.194	5.392
4	9.195	8.881	8.989	8.881	8.806	8.748	9.323
5	8.940	8.698	8.567	8.394	8.274	8.179	8.298
6	11.628	11.516	11.047	10.860	10.763	10.702	11.260
7	14.716	14.747	14.188	14.114	14.102	14.104	14.534
8	14.300	14.011	13.864	13.612	13.418	13.256	13.618
9	17.598	17.511	16.815	16.541	16.394	16.297	17.423
10	21.525	21.651	20.881	20.804	20.803	20.817	21.565
11	5.360	4.992	5.204	5.216	5.240	5.262	5.139
12	7.787	7.363	7.593	7.596	7.617	7.638	7.646
13	6.204	6.143	6.066	6.010	5.972	5.943	5.986
14	8.190	8.183	8.010	7.976	7.968	7.968	8.152
15	10.409	10.483	10.268	10.279	10.298	10.316	10.487
16	10.826	10.644	10.631	10.569	10.530	10.499	10.360
17	13.174	13.074	12.885	12.830	12.819	12.820	12.968
18	15.803	15.837	15.575	15.579	15.603	15.629	15.760
19	4.459	4.150	4.335	4.355	4.383	4.408	4.341
20	6.184	5.835	6.021	6.036	6.064	6.091	6.113
21	7.596	6.838	6.763	6.689	6.702	6.728	6.561
22	8.170	7.036	7.686	7.665	7.701	7.743	6.828
23	6.277	6.734	6.397	6.725	6.998	7.213	6.746
24	7.018	6.920	6.988	7.109	7.182	7.227	6.767
25	7.511	7.103	6.922	6.946	7.033	7.117	7.434
26	8.928	7.967	8.046	7.960	7.972	8.000	7.902
27	8.265	7.793	7.946	7.967	8.022	8.083	7.881
28	5.083	7.806	6.601	7.442	7.990	8.372	7.640
29	7.770	7.672	7.771	7.946	8.052	8.119	7.726
30	9.561	9.137	9.302	9.403	9.477	9.528	9.394
31	6.164	6.010	6.072	6.069	6.066	6.063	5.999
32	7.882	7.799	7.768	7.779	7.791	7.802	7.899
33	9.864	9.800	9.794	9.817	9.836	9.852	9.789
34	10.080	9.854	9.906	9.890	9.882	9.874	9.752
35	12.001	11.856	11.793	11.788	11.797	11.808	11.814
36	14.219	14.103	14.062	14.072	14.089	14.105	14.000
MAE (17 IPs)	0.248	0.206	0.251	0.271	0.297	0.324	
MAE (35 IPs)	0.364	0.170	0.238	0.216	0.247	0.284	

†Reference [2]

Table S5 Δ-SCF ionization potentials (in eV) for OSIC(w,k) where $k = 1-3$ with LSDA.

Z	OSIC(w)			$E^{\dagger}_{Exp}$
	$k=1$	$k=2$	$k=3$	
2	25.032	25.032	25.032	24.587
3	5.454	5.409	5.376	5.392
4	9.076	9.009	8.959	9.323
5	8.730	8.613	8.525	8.298
6	11.216	11.044	10.946	11.26
7	14.389	14.300	14.274	14.534
8	14.161	14.025	13.901	13.618
9	17.101	16.881	16.749	17.423
10	21.188	21.108	21.095	21.565
11	5.316	5.318	5.322	5.139
12	7.717	7.714	7.718	7.646
13	6.149	6.125	6.108	5.986
14	8.077	8.033	8.011	8.152
15	10.329	10.310	10.309	10.487
16	10.770	10.747	10.728	10.36
17	12.984	12.918	12.888	12.968
18	15.659	15.629	15.628	15.76
19	4.444	4.453	4.462	4.341
20	6.155	6.165	6.176	6.113
21	7.182	7.100	7.068	6.561
22	7.835	7.786	7.788	6.828
23	6.412	6.619	6.811	6.746
24	7.165	7.231	7.265	6.767
25	7.246	7.258	7.289	7.434
26	8.499	8.402	8.358	7.902
27	8.172	8.162	8.165	7.881
28	6.761	7.567	8.060	7.64
29	7.946	8.038	8.088	7.726
30	9.515	9.497	9.482	9.394
31	6.131	6.131	6.130	5.999
32	7.860	7.865	7.872	7.899
33	9.853	9.856	9.863	9.789
34	10.031	10.028	10.022	9.752
35	11.922	11.918	11.923	11.814
36	14.148	14.142	14.150	14
MAE (17 IPs)	0.223	0.247	0.255	
MAE (35 IPs)	0.267	0.247	0.259	

†Reference [2]

Table S6 Δ-SCF electron affinities (in eV) for PZSIC, LSIC(z), and LSIC(w,k) where $k = 1-4$ with LSDA.

Z	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Exp}$
		$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
1	0.715	0.715	0.715	0.715	0.715	0.715	0.754
3	0.553	0.490	0.491	0.450	0.420	0.395	0.618
5	0.235	0.425	0.027	-0.013	-0.024	-0.027	0.280
6	1.114	1.418	0.984	1.026	1.068	1.102	1.262
8	1.065	1.360	0.737	0.640	0.594	0.565	1.462
9	2.888	3.376	2.716	2.785	2.855	2.913	3.401
11	0.582	0.470	0.533	0.534	0.540	0.548	0.548
13	0.312	0.479	0.294	0.310	0.327	0.343	0.434
14	1.236	1.443	1.247	1.296	1.332	1.358	1.390
15	0.917	0.964	0.859	0.830	0.807	0.788	0.747
16	2.061	2.166	1.954	1.950	1.964	1.980	2.077
17	3.490	3.696	3.439	3.486	3.530	3.566	3.613
19	0.540	0.425	0.480	0.484	0.493	0.503	0.501
22	-1.247	-0.080	-1.097	-0.786	-0.561	-0.400	0.087
29	1.312	1.123	1.181	1.260	1.316	1.354	1.236
31	0.178	0.302	0.261	0.286	0.300	0.311	0.43
32	1.208	1.297	1.273	1.312	1.336	1.352	1.233
33	0.969	0.956	0.922	0.920	0.915	0.910	0.814
34	2.068	2.089	1.985	1.999	2.015	2.028	2.021
35	3.405	3.479	3.406	3.453	3.484	3.505	3.364
MAE (12 EAs)	0.152	0.097	0.235	0.229	0.215	0.202	
MAE (20 EAs)	0.190	0.102	0.224	0.205	0.189	0.176	

†Reference [3]

Table S7 Δ-SCF electron affinities (in eV) for OSIC(w,k) where $k = 1-3$ with LSDA.

Z	OSIC(w)			$E^{\dagger}_{Exp}$
	$k=1$	$k=2$	$k=3$	
1	0.715	0.715	0.715	0.754
3	0.519	0.498	0.481	0.618
5	0.165	0.134	0.120	0.280
6	1.137	1.165	1.194	1.262
8	0.998	0.944	0.908	1.462
9	2.996	3.062	3.120	3.401
11	0.563	0.562	0.564	0.548
13	0.333	0.343	0.352	0.434
14	1.289	1.314	1.333	1.390
15	0.962	0.976	0.982	0.747
16	2.035	2.026	2.025	2.077
17	3.511	3.530	3.552	3.613
19	0.531	0.533	0.536	0.501
22	-0.871	-0.653	-0.495	0.087
29	1.278	1.258	1.242	1.236
31	0.298	0.328	0.345	0.43
32	1.299	1.330	1.349	1.233
33	1.014	1.039	1.050	0.814
34	2.100	2.121	2.137	2.021
35	3.477	3.517	3.545	3.364
MAE (12 EAs)	0.152	0.150	0.145	
MAE (20 EAs)	0.172	0.164	0.155	

†Reference [3]

Table S8 Atomization energies of selected molecules (in kJ/mol) for PZSIC, LSIC(z), and LSIC(w).

System	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Exp}$
		$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
HF	609.4	603.6	568.7	562.7	560.4	559.0	566.6
LiF	558.1	557.6	513.7	509.4	507.8	506.1	575.6
F_2	189.9	150.8	204.8	222.2	230.9	235.7	154.5
HCl	490.4	460.5	455.8	447.1	442.6	439.6	427.8
LiCl	465.3	452.5	437.9	433.7	432.2	431.1	472.9
NaCl	394.6	394.5	379.6	381.6	384.8	387.7	407.4
Cl_2	299.2	234.7	275.9	283.0	288.6	292.8	239.3
HBr	442.6	398.2	405.8	394.6	388.2	384.1	362.4
LiBr	425.9	400.5	401.8	397.1	394.5	392.5	425.1
NaBr	367.8	352.0	355.6	355.5	356.5	357.7	363.3
FBr	298.4	241.7	273.3	281.9	288.8	293.8	246.4
Br_2	271.8	204.1	251.2	254.2	257.0	259.3	190.2
C_6H_6	6341.0	5631.3	5758.8	5571.1	5444.0	5345.5	5463
C_4H_4O	4627.8	4114.4	4125.6	4000.8	3923.2	3863.5	3977.4
C_4H_6	4673.0	4236.9	4200.6	4052.4	3957.4	3884.8	3982
C_2H_6	3354.3	3051.3	3038.8	2930.6	2860.0	2806.4	2787
N_2	985.1	924.6	922.9	891.2	863.6	838.5	941.6
N_2H_4	2128.9	1883.1	1892.8	1804.1	1742.3	1693.4	1696.4
H_2	479.2	479.2	479.2	479.2	479.2	479.2	432.1
H_2O_2	1241.7	1128.8	1108.4	1075.3	1054.9	1039.6	1055.5
BeH	261.6	238.7	240.2	230.7	224.0	218.6	216.8
BH_3	1321.5	1223.7	1221.3	1179.7	1151.6	1129.8	1116.1
$C_2H_2O_2$	2891.8	2615.8	2605.1	2534.3	2488.6	2452.4	2554.5
C_3H_4	3257.8	2981.0	2933.1	2828.9	2761.4	2709.4	2806.1
C_4H_8	5483.4	4878.0	4913.1	4733.7	4618.7	4531.9	4520.1
S_2	457.3	413.4	443.9	454.7	463.4	470.3	421.6
SiH_4	1524.6	1380.2	1435.2	1400.4	1376.1	1357.0	1265.9
SiO	761.1	738.3	713.8	716.1	719.3	721.4	794.1
SO_2	1027.1	934.8	933.1	937.9	943.8	947.6	1062.9
O_2	487.6	469.5	464.4	467.4	468.0	467.2	493.7
CO	1071.5	1036.7	1000.2	987.4	978.8	971.1	1071.8
CO_2	1535.2	1457.0	1366.5	1346.1	1342.2	1341.2	1598
C_2H_2	1823.8	1716.4	1657.3	1600.5	1562.3	1532.0	1626.5
Li_2	92.2	72.8	69.8	57.9	48.7	41.0	100
CH_4	1952.4	1815.4	1787.0	1725.2	1684.0	1652.3	1642
NH_3	1392.8	1293.3	1260.1	1205.4	1167.7	1138.2	1157.9
H_2O	1029.5	992.7	930.5	900.8	883.4	871.1	917.8
MAE	196.0	83.8	91.6	61.8	53.1	58.0	

†Reference [3]

Table S9 Atomization energies of selected molecules (in kJ/mol) for OSIC(w) with LSDA.

System	OSIC(w)			$E^{\dagger}_{Exp}$
	$k=1$	$k=2$	$k=3$	
HF	590.4	585.6	584.1	566.6
LiF	549.1	547.7	548.0	575.6
F_2	227.7	243.5	251.8	154.5
HCl	470.6	463.8	459.9	427.8
LiCl	456.5	453.8	452.8	472.9
NaCl	392.2	393.1	394.9	407.4
Cl_2	293.3	295.0	296.4	239.3
HBr	422.7	414.8	409.9	362.4
LiBr	421.8	420.3	419.5	425.1
NaBr	369.0	369.7	370.8	363.3
FBr	302.9	308.6	312.8	246.4
Br_2	269.1	269.7	270.4	190.2
C_6H_6	6111.5	5998.9	5920.5	5463
C_4H_4O	4402.7	4321.2	4269.9	3977.4
C_4H_6	4442.8	4350.8	4291.5	3982
C_2H_6	3190.8	3124.5	3080.8	2787
N_2	977.4	961.2	944.2	941.6
N_2H_4	2015.0	1960.8	1920.4	1696.4
H_2	479.2	479.2	479.2	432.1
H_2O_2	1179.1	1154.4	1138.2	1055.5
BeH	252.1	247.0	243.2	216.8
BH_3	1268.3	1243.2	1225.9	1116.1
$C_2H_2O_2$	2766.7	2718.9	2687.5	2554.5
C_3H_4	3101.7	3036.7	2994.5	2806.1
C_4H_8	5198.3	5086.7	5014.1	4520.1
S_2	459.3	462.5	465.0	421.6
SiH_4	1478.6	1459.8	1446.3	1265.9
SiO	758.0	759.5	760.9	794.1
SO_2	1007.1	1005.9	1005.7	1062.9
O_2	493.3	495.0	495.1	493.7
CO	1049.6	1040.9	1035.3	1071.8
CO_2	1493.8	1489.6	1491.4	1598
C_2H_2	1749.2	1713.8	1690.1	1626.5
Li_2	81.7	77.2	74.0	100
CH_4	1864.7	1827.9	1803.3	1642
NH_3	1325.0	1292.1	1268.2	1157.9
H_2O	974.2	953.3	941.0	917.8
MAE	144.6	122.5	107.5	

†Reference [3]

Table S10 Barrier heights for BH6 set of data (in kcal/mol) for PZSIC, LSIC(z), and LSIC(w) methods.

Reaction	Direction	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Ref}$
			$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
$OH + CH_4 \rightarrow CH_3 + H_2O$	Forward	4.5	9.3	8.0	7.7	7.0	6.2	6.7
	Reverse	7.2	19.4	11.6	13.2	14.1	14.7	19.6
$H + OH \rightarrow H_2 + O$	Forward	9.6	10.1	5.4	3.7	2.8	2.3	10.7
	Reverse	8.5	14.3	17.1	20.3	22.4	24.1	13.1
$H + H_2S \rightarrow H_2 + HS$	Forward	1.9	2.3	3.0	3.0	2.9	2.9	3.6
	Reverse	10.3	19.5	19.9	22.4	23.8	24.7	17.3
ME		-4.8	0.7	-1.0	-0.1	0.3	0.6	
MAE		4.8	1.3	3.6	4.6	5.0	5.5	

†Reference [4]

Table S11 Barrier heights for BH6 set of data (in kcal/mol) for OSIC(w) method.

Reaction	Direction	OSIC(w)			$E^{\dagger}_{Ref}$
		$k=1$	$k=2$	$k=3$	
$OH + CH_4 \rightarrow CH_3 + H_2O$	Forward	4.4	3.8	3.2	6.7
	Reverse	7.9	7.7	7.7	19.6
$H + OH \rightarrow H_2 + O$	Forward	7.2	5.9	5.2	10.7
	Reverse	13.7	16.1	17.8	13.1
$H + H_2S \rightarrow H_2 + HS$	Forward	2.3	2.0	1.7	3.6
	Reverse	15.3	16.7	17.5	17.3
ME		-3.4	-3.1	-3.0	
MAE		3.6	4.1	4.6	

†Reference [4]

Table S12 Reaction energies for SIE11 set of data (in kcal/mol) for PZSIC, LSIC(z), and LSIC(w) methods.

Reaction	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Ref}$
		$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
$He_2^+ \rightarrow He + He^+$	62.74	55.19	56.86	54.16	52.23	50.67	56.9
$(NH3)_2^+ \rightarrow NH_3 + NH_3^+$	47.60	37.53	44.51	43.38	42.57	42.02	35.9
$(H2O)_2^+ \rightarrow H_2O + H_2O^+$	45.65	40.07	49.64	51.20	51.67	51.86	39.7
$C_4H_{10}^+ \rightarrow C_2H_5 + C_2H_5^+$	46.72	29.29	41.40	42.27	42.97	43.49	35.28
$(CH3)_2CO^+ \rightarrow CH_3 + CH_3CO^+$	61.96	24.43	41.05	35.54	32.62	30.90	22.57
$ClFCl \rightarrow ClClF^+$	-3.61	-3.36	-6.52	-8.15	-9.18	-9.96	-1.01
$C_2H_4...F_2 \rightarrow C_2H_4 + F_2$	0.85	-1.74	0.39	0.75	1.04	1.27	1.08
$C_6H_6...Li \rightarrow Li + C_6H_6$	19.69	-4.00	13.18	7.69	3.48	0.31	9.50
$NH_3...ClF \rightarrow NH_3 + ClF$	16.11	5.94	11.78	12.20	12.78	13.32	10.50
$NaOMg \rightarrow MgO + Na$	98.36	81.01	83.58	79.30	77.16	75.88	69.56
$FLiF \rightarrow Li + F_2$	89.54	93.18	71.60	65.48	62.66	60.93	94.36
MAE	11.51	4.31	8.28	8.30	8.81	9.27	

†Reference [5]

Table S13 Reaction energies for SIE11 set of data (in kcal/mol) for OSIC(w) method.

Reaction	OSIC(w)			$E^{\dagger}_{Ref}$
	$k=1$	$k=2$	$k=3$	
$He_2^+ \rightarrow He + He^+$	59.93	58.53	57.47	56.9
$(NH_3)_2^+ \rightarrow NH_3 + NH_3^+$	48.88	49.29	49.47	35.9
$(H_2O)_2^+ \rightarrow H_2O + H_2O^+$	52.25	54.11	54.87	39.7
$C_4H_{10}^+ \rightarrow C_2H_5 + C_2H_5^+$	46.99	48.18	49.00	35.28
$(CH_3)_2CO^+ \rightarrow CH_3 + CH_3CO^+$	50.57	47.76	46.10	22.57
$ClFCl \rightarrow ClClF$	-7.57	-9.32	-10.34	-1.01
$C_2H_4...F_2 \rightarrow C_2H_4 + F_2$	1.25	1.51	1.67	1.08
$C_6H_6...Li \rightarrow Li + C_6H_6$	17.56	14.67	12.50	9.50
$NH_3...ClF \rightarrow NH_3 + ClF$	16.14	16.61	16.87	10.50
$NaOMg \rightarrow MgO + Na$	86.99	83.22	81.28	69.56
$FLiF \rightarrow Li + F_2$	78.02	74.18	72.48	94.36
MAE	11.13	11.03	10.86	

†Reference [5]

Table S14 Dissociation energies for SIE4x4 set of data (in kcal/mol) for PZSIC, LSIC(z), and LSIC(w) methods.

Reaction	R/R_e	PZSIC	LSIC(z)	LSIC(w)				$E^{\dagger}_{Ref}$
			$k=1$	$k=1$	$k=2$	$k=3$	$k=4$	
$H_2^+ \rightarrow H + H^+$	1.0	64.4	64.4	64.4	64.4	64.4	64.4	64.4
	1.25	58.9	58.9	58.9	58.9	58.9	58.9	58.9
	1.5	48.7	48.7	48.7	48.7	48.7	48.7	48.7
	1.75	38.2	38.2	38.2	38.2	38.2	38.2	38.3
$He_2^+ \rightarrow He + He^+$	1.0	62.7	55.2	56.9	54.2	52.2	50.7	56.9
	1.25	48.8	44.2	45.4	43.9	42.7	41.8	46.9
	1.5	30.9	28.3	29.0	28.2	27.5	27.0	31.3
	1.75	17.5	16.1	16.5	16.1	15.7	15.4	19.1
$(NH_3)_2^+ \rightarrow NH_3 + NH_3^+$	1.0	47.6	37.5	44.5	43.4	42.6	42.0	35.9
	1.25	33.3	32.6	39.0	39.5	39.0	38.4	25.9
	1.5	17.5	21.5	26.2	27.4	27.2	26.8	13.4
	1.75	8.4	11.6	13.7	14.1	13.9	13.5	4.9
$(H_2O)_2^+ \rightarrow H_2O + H_2O^+$	1.0	45.7	40.1	49.6	51.2	51.7	51.9	39.7
	1.25	27.8	33.3	39.2	42.0	42.9	43.2	29.1
	1.5	14.4	18.4	20.0	21.3	21.9	22.2	16.9
	1.75	8.0	11.1	11.2	12.1	12.4	12.7	9.3
MAE		3.0	2.6	4.7	5.5	5.8	5.9	

†Reference [6]

Table S15 Dissociation energies for SIE4x4 set of data (in kcal/mol) for OSIC(w) method (kcal/mol).

Reaction	R/R_e	OSIC(w)			$E^{\dagger}_{Ref}$
		$k=1$	$k=2$	$k=3$	
$H_2^+ \rightarrow H + H^+$	1.0	64.4	64.4	64.4	64.4
	1.25	58.9	58.9	58.9	58.9
	1.5	48.7	48.7	48.7	48.7
	1.75	38.2	38.2	38.2	38.3
$He_2^+ \rightarrow He + He^+$	1.0	59.9	58.5	57.5	56.9
	1.25	47.3	46.5	45.9	46.9
	1.5	30.1	29.7	29.4	31.3
	1.75	17.1	16.9	16.7	19.1
$(NH_3)_2^+ \rightarrow NH_3 + NH_3^+$	1.0	48.9	49.3	49.5	35.9
	1.25	39.9	41.6	42.2	25.9
	1.5	25.9	28.1	29.1	13.4
	1.75	13.5	15.1	15.8	4.9
$(H_2O)_2^+ \rightarrow H_2O + H_2O^+$	1.0	52.3	54.1	54.9	39.7
	1.25	39.4	42.8	44.3	29.1
	1.5	20.1	22.0	22.9	16.9
	1.75	11.3	12.6	13.3	9.3
MAE		5.2	6.0	6.4	

†Reference [6]

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