Encapsulation of hydrogen molecule in C_{50} fullerene: an *ab initio* study of structural, energetic and electronic properties of $H_2@C_{50}$ and $2H_2@C_{50}$ complexes

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Supporting Materials

C50 from MP2(fc)/6-311G(d,p)

C	0.000000	1.238325	2.687486
C	-1.177717	0.382664	2.687486
C	-0.727869	-1.001826	2.687486
C	0.727869	-1.001826	2.687486
C	1.177717	0.382664	2.687486
C	0.000000	1.238325	-2.687486
C	-1.177717	0.382664	-2.687486
C	-0.727869	-1.001826	-2.687486
C	0.727869	-1.001826	-2.687486
C	1.177717	0.382664	-2.687486
C	0.000000	2.467449	1.996830
C	-2.346684	0.762484	1.996830
C	-1.450330	-1.996209	1.996830
C	1.450330	-1.996209	1.996830
C	2.346684	0.762484	1.996830
C	0.000000	2.467449	-1.996830
C	-2.346684	0.762484	-1.996830
C	-1.450330	-1.996209	-1.996830
C	1.450330	-1.996209	-1.996830
C	2.346684	0.762484	-1.996830
C	-1.189339	2.847818	1.241788
C	-3.075962	-0.251104	1.241788
C	-0.711710	-3.003009	1.241788
C	2.636101	-1.604857	1.241788
C	2.340910	2.011153	1.241788
C	-1.189339	2.847818	-1.241788
C	-3.075962	-0.251104	-1.241788
C	-0.711710	-3.003009	-1.241788
C	2.636101	-1.604857	-1.241788
C	2.340910	2.011153	-1.241788
C	1.189339	2.847818	-1.241788
C	-2.340910	2.011153	-1.241788
C	-2.636101	-1.604857	-1.241788
C	0.711710	-3.003009	-1.241788
C	3.075962	-0.251104	-1.241788
C	1.189339	2.847818	1.241788
C	-2.340910	2.011153	1.241788
C	-2.636101	-1.604857	1.241788
C	0.711710	-3.003009	1.241788
C	3.075962	-0.251104	1.241788
C	-0.731933	3.380527	0.000000
C	-3.441252	0.348531	0.000000
C	-1.394878	-3.165123	0.000000

C	2.579170	-2.304684	0.000000
C	2.988892	1.740750	0.000000
C	0.731933	3.380527	0.000000
C	-2.988892	1.740750	0.000000
C	-2.579170	-2.304684	0.000000
C	1.394878	-3.165123	0.000000
C	3.441252	0.348531	0.000000

H2@C50 from MP2(fc)/6-311G(d,p)

H	0.281690	-0.162428	0.000000
H	-0.374650	0.179524	0.000000
C	1.243754	-2.686812	0.000000
C	0.388327	-2.688692	1.177636
C	-0.995187	-2.691724	0.728023
C	-0.995187	-2.691724	-0.728023
C	0.388327	-2.688692	-1.177636
C	1.231644	2.691647	0.000000
C	0.376266	2.690049	1.177410
C	-1.007688	2.688731	0.728125
C	-1.007688	2.688731	-0.728125
C	0.376266	2.690049	-1.177410
C	2.471457	-1.993656	0.000000
C	0.766308	-1.995830	2.346212
C	-1.989421	-2.000858	1.450623
C	-1.989421	-2.000858	-1.450623
C	0.766308	-1.995830	-2.346212
C	2.461255	2.001050	0.000000
C	0.757268	1.998686	2.345874
C	-1.999641	1.993459	1.450517
C	-1.999641	1.993459	-1.450517
C	0.757268	1.998686	-2.345874
C	2.849736	-1.236985	1.188418
C	-0.247461	-1.241919	3.075193
C	-2.996388	-1.248089	0.711434
C	-1.600764	-1.244168	-2.635449
C	2.012509	-1.238272	-2.338905
C	2.843216	1.247098	1.188249
C	-0.253117	1.240912	3.074721
C	-3.003170	1.236017	0.711544
C	-1.606700	1.239006	-2.635470
C	2.006513	1.245774	-2.338649
C	2.843216	1.247098	-1.188249
C	2.006513	1.245774	2.338649
C	-1.606700	1.239006	2.635470
C	-3.003170	1.236017	-0.711544

C	-0.253117	1.240912	-3.074721
C	2.849736	-1.236985	-1.188418
C	2.012509	-1.238272	2.338905
C	-1.600764	-1.244168	2.635449
C	-2.996388	-1.248089	-0.711434
C	-0.247461	-1.241919	-3.075193
C	3.380830	0.006158	0.731688
C	0.349824	0.000651	3.441594
C	-3.164086	-0.006574	1.394942
C	-2.304673	-0.004315	-2.579501
C	1.741190	0.003347	-2.988368
C	3.380830	0.006158	-0.731688
C	1.741190	0.003347	2.988368
C	-2.304673	-0.004315	2.579501
C	-3.164086	-0.006574	-1.394942
C	0.349824	0.000651	-3.441594

2H2@C50 from MP2(fc)/6-311G(d,p)

H	-0.380155	-0.924797	0.000000
H	0.344257	-1.046681	0.000000
H	-0.376377	0.949929	0.000000
H	0.356698	1.001132	0.000000
C	-0.475504	1.148283	2.692181
C	-1.228729	-0.099863	2.688239
C	-0.286436	-1.211116	2.693140
C	1.053397	-0.646446	2.688933
C	0.937067	0.807844	2.689470
C	-0.475504	1.148283	-2.692181
C	-1.228729	-0.099863	-2.688239
C	-0.286436	-1.211116	-2.693140
C	1.053397	-0.646446	-2.688933
C	0.937067	0.807844	-2.689470
C	-0.946527	2.290770	2.004625
C	-2.450749	-0.198995	1.995117
C	-0.570369	-2.415450	2.006936
C	2.099912	-1.289155	1.996565
C	1.867358	1.612178	1.998137
C	-0.946527	2.290770	-2.004625
C	-2.450749	-0.198995	-1.995117
C	-0.570369	-2.415450	-2.006936
C	2.099912	-1.289155	-1.996565
C	1.867358	1.612178	-1.998137
C	-2.186074	2.176977	1.243265
C	-2.733526	-1.416601	1.241430
C	0.496975	-3.066212	1.248494

C	3.038369	-0.467920	1.240534
C	1.386960	2.770827	1.246156
C	-2.186074	2.176977	-1.243265
C	-2.733526	-1.416601	-1.241430
C	0.496975	-3.066212	-1.248494
C	3.038369	-0.467920	-1.240534
C	1.386960	2.770827	-1.246156
C	0.001963	3.108041	-1.248655
C	-2.922806	0.957440	-1.240871
C	-1.811928	-2.503341	-1.244472
C	1.809238	-2.508631	-1.244734
C	2.924525	0.951892	-1.240833
C	0.001963	3.108041	1.248655
C	-2.922806	0.957440	1.240871
C	-1.811928	-2.503341	1.244472
C	1.809238	-2.508631	1.244734
C	2.924525	0.951892	1.240833
C	-1.969797	2.846241	0.000000
C	-3.300075	-1.001786	0.000000
C	-0.070653	-3.476506	0.000000
C	3.255577	-1.136115	0.000000
C	2.087116	2.765148	0.000000
C	-0.623882	3.420495	0.000000
C	-3.416285	0.457595	0.000000
C	-1.491218	-3.128783	0.000000
C	2.500040	-2.390428	0.000000
C	3.032202	1.646499	0.000000