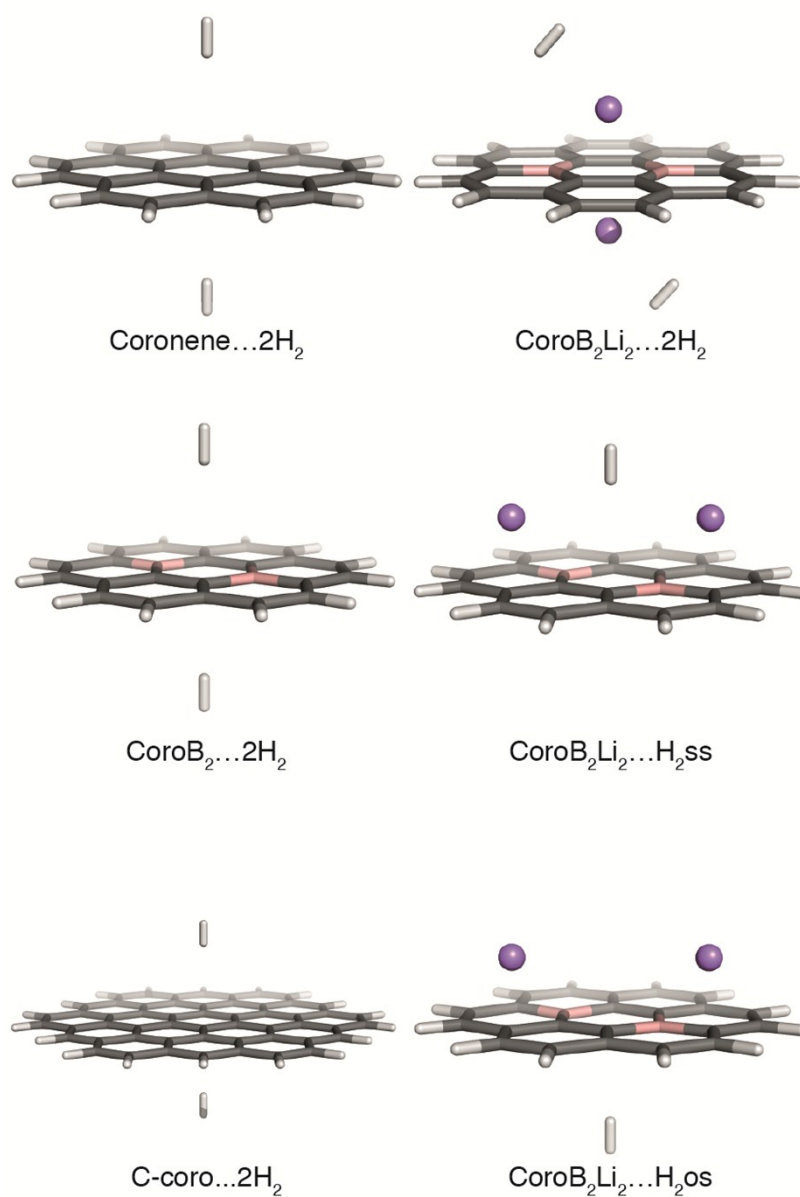


Supporting Information

Choosing a Density Functional for Modeling Adsorptive Hydrogen Storage: Reference Quantum Mechanical Calculations and a Comparison of Dispersion-Corrected Density Functionals

Mikuláš Kocman, Petr Jurečka, Matúš Dubecký, Michal Otyepka, Yeonchoo Cho,
Kwang S. Kim



Coronene...2H₂

C	-1.2346511	-0.7128261	0.0000000
C	-1.2346511	0.7128261	0.0000000
C	0.0000000	1.4256523	0.0000000
C	1.2346511	0.7128261	0.0000000
C	1.2346511	-0.7128261	0.0000000
C	0.0000000	-1.4256523	0.0000000
C	-2.4670697	1.4244034	0.0000000
C	0.0000000	2.8487267	0.0000000
C	-1.2469441	3.5331924	0.0000000
C	-2.4403623	2.8464814	0.0000000
C	-2.4670697	-1.4244034	0.0000000
C	-3.6833064	-0.6867110	0.0000000
C	-3.6833064	0.6867110	0.0000000
C	-2.4403623	-2.8464814	0.0000000
C	-1.2469441	-3.5331924	0.0000000
C	0.0000000	-2.8487267	0.0000000
C	1.2469441	-3.5331924	0.0000000
C	2.4403623	-2.8464814	0.0000000
C	2.4670697	-1.4244034	0.0000000
C	3.6833064	-0.6867110	0.0000000
C	3.6833064	0.6867110	0.0000000
C	2.4670697	1.4244034	0.0000000
C	2.4403623	2.8464814	0.0000000
C	1.2469441	3.5331924	0.0000000
H	-1.2440968	4.6195959	0.0000000
H	-3.3786390	3.3872174	0.0000000
H	-4.6227358	-1.2323785	0.0000000
H	-4.6227358	1.2323785	0.0000000
H	-3.3786390	-3.3872174	0.0000000
H	-1.2440968	-4.6195959	0.0000000
H	1.2440968	-4.6195959	0.0000000
H	3.3786390	-3.3872174	0.0000000
H	4.6227358	-1.2323785	0.0000000
H	4.6227358	1.2323785	0.0000000
H	3.3786390	3.3872174	0.0000000
H	1.2440968	4.6195959	0.0000000
H	0.0000000	0.0000000	3.4710000
H	0.0000000	0.0000000	2.7290000
H	0.0000000	0.0000000	-2.7290000
H	0.0000000	0.0000000	-3.4710000

CoroB₂...2H₂

B	-1.5875542	0.0000000	0.0000000
C	-0.6762146	0.0000000	-1.2524544
C	0.6762146	0.0000000	-1.2524544
B	1.5875542	0.0000000	0.0000000
C	0.6762146	0.0000000	1.2524544
C	-0.6762146	0.0000000	1.2524544
C	-1.4952689	0.0000000	2.4412557
C	-2.9141535	0.0000000	2.4308574
C	-3.6823871	0.0000000	1.2802070
C	-3.0552729	0.0000000	0.0000000
C	-3.6823871	0.0000000	-1.2802070
C	-2.9141535	0.0000000	-2.4308574
C	-1.4952689	0.0000000	-2.4412557
C	-0.6831736	0.0000000	-3.6269340
C	0.6831736	0.0000000	-3.6269340
C	1.4952689	0.0000000	-2.4412557
C	2.9141535	0.0000000	-2.4308574
C	3.6823871	0.0000000	-1.2802070
C	3.0552729	0.0000000	0.0000000
C	3.6823871	0.0000000	1.2802070
C	2.9141535	0.0000000	2.4308574
C	1.4952689	0.0000000	2.4412557
C	0.6831736	0.0000000	3.6269340
C	-0.6831736	0.0000000	3.6269340
H	-3.4136162	0.0000000	3.3952876
H	-4.7662323	0.0000000	1.3719596
H	-4.7662323	0.0000000	-1.3719596
H	-3.4136162	0.0000000	-3.3952876
H	-1.2162584	0.0000000	-4.5755905
H	1.2162584	0.0000000	-4.5755905
H	3.4136162	0.0000000	-3.3952876
H	4.7662323	0.0000000	-1.3719596
H	4.7662323	0.0000000	1.3719596
H	3.4136162	0.0000000	3.3952876
H	1.2162584	0.0000000	4.5755905
H	-1.2162584	0.0000000	4.5755905
H	0.0000000	2.7334350	0.0000000
H	0.0000000	3.4754350	0.0000000
H	0.0000000	-2.7334350	0.0000000
H	0.0000000	-3.4754350	0.0000000

C-coro...2H₂

C	-1.2288787	-0.7094934	0.0000000
C	-1.2288787	0.7094934	0.0000000
C	0.0000000	1.4189869	0.0000000
C	1.2288787	0.7094934	0.0000000
C	1.2288787	-0.7094934	0.0000000
C	0.0000000	-1.4189869	0.0000000
C	-2.4632768	-1.4221735	0.0000000
C	-2.4618561	-2.8419276	0.0000000
C	-1.2302535	-3.5529937	0.0000000
C	0.0000000	-2.8443471	0.0000000
C	1.2302535	-3.5529937	0.0000000
C	2.4618561	-2.8419276	0.0000000
C	2.4632768	-1.4221735	0.0000000
C	3.6921095	-0.7110661	0.0000000
C	3.6921095	0.7110661	0.0000000
C	2.4632768	1.4221735	0.0000000
C	2.4618561	2.8419276	0.0000000
C	1.2302535	3.5529937	0.0000000
C	0.0000000	2.8443471	0.0000000
C	-1.2302535	3.5529937	0.0000000
C	-2.4618561	2.8419276	0.0000000
C	-2.4632768	1.4221735	0.0000000
C	-3.6921095	0.7110661	0.0000000
C	-3.6921095	-0.7110661	0.0000000
C	-3.7034231	-3.5523899	0.0000000
C	-1.2247484	-4.9834534	0.0000000
C	1.2247484	-4.9834534	0.0000000
C	3.7034231	-3.5523899	0.0000000
C	4.9281715	-1.4310635	0.0000000
C	4.9281715	1.4310635	0.0000000
C	3.7034231	3.5523899	0.0000000
C	1.2247484	4.9834534	0.0000000
C	-1.2247484	4.9834534	0.0000000
C	-3.7034231	3.5523899	0.0000000
C	-4.9281715	1.4310635	0.0000000
C	-4.9281715	-1.4310635	0.0000000
C	0.0000000	5.6634589	0.0000000
C	2.4844343	5.6676017	0.0000000
C	3.6657635	4.9851840	0.0000000
C	4.9046993	2.8317695	0.0000000
C	6.1501578	0.6820177	0.0000000
C	6.1501578	-0.6820177	0.0000000
C	4.9046993	-2.8317695	0.0000000
C	3.6657635	-4.9851840	0.0000000
C	2.4844343	-5.6676017	0.0000000
C	0.0000000	-5.6634589	0.0000000
C	-2.4844343	-5.6676017	0.0000000

C	-3.6657635	-4.9851840	0.0000000
C	-4.9046993	-2.8317695	0.0000000
C	-6.1501578	-0.6820177	0.0000000
C	-6.1501578	0.6820177	0.0000000
C	-4.9046993	2.8317695	0.0000000
C	-3.6657635	4.9851840	0.0000000
C	-2.4844343	5.6676017	0.0000000
H	0.0000000	6.7508036	0.0000000
H	2.4839236	6.7531766	0.0000000
H	4.6064607	5.5277692	0.0000000
H	5.8463674	3.3754018	0.0000000
H	7.0903843	1.2254474	0.0000000
H	7.0903843	-1.2254474	0.0000000
H	5.8463674	-3.3754018	0.0000000
H	4.6064607	-5.5277692	0.0000000
H	2.4839236	-6.7531766	0.0000000
H	0.0000000	-6.7508036	0.0000000
H	-2.4839236	-6.7531766	0.0000000
H	-4.6064607	-5.5277692	0.0000000
H	-5.8463674	-3.3754018	0.0000000
H	-7.0903843	-1.2254474	0.0000000
H	-7.0903843	1.2254474	0.0000000
H	-5.8463674	3.3754018	0.0000000
H	-4.6064607	5.5277692	0.0000000
H	-2.4839236	6.7531766	0.0000000
H	0.0000000	0.0000000	3.4710000
H	0.0000000	0.0000000	2.7290000
H	0.0000000	0.0000000	-2.7290000
H	0.0000000	0.0000000	-3.4710000

CoroB₂Li₂...2H₂

B	-1.4901158	0.0000000	0.0000000
C	-0.7214808	0.0000000	-1.3201461
C	0.7214808	0.0000000	-1.3201461
B	1.4901158	0.0000000	0.0000000
C	0.7214808	0.0000000	1.3201461
C	-0.7214808	0.0000000	1.3201461
C	-1.4590995	0.0000000	2.5442482
C	-2.8895583	0.0000000	2.4720350
C	-3.6194194	0.0000000	1.2822650
C	-2.9942746	0.0000000	0.0000000
C	-3.6194194	0.0000000	-1.2822650
C	-2.8895583	0.0000000	-2.4720350
C	-1.4590995	0.0000000	-2.5442482
C	-0.6939531	0.0000000	-3.7516112
C	0.6939531	0.0000000	-3.7516112
C	1.4590995	0.0000000	-2.5442482
C	2.8895583	0.0000000	-2.4720350
C	3.6194194	0.0000000	-1.2822650
C	2.9942746	0.0000000	0.0000000
C	3.6194194	0.0000000	1.2822650
C	2.8895583	0.0000000	2.4720350
C	1.4590995	0.0000000	2.5442482
C	0.6939531	0.0000000	3.7516112
C	-0.6939531	0.0000000	3.7516112
H	-3.4411050	0.0000000	3.4100551
H	-4.7073598	0.0000000	1.3630236
H	-4.7073598	0.0000000	-1.3630236
H	-3.4411050	0.0000000	-3.4100551
H	-1.2161081	0.0000000	-4.7060517
H	1.2161081	0.0000000	-4.7060517
H	3.4411050	0.0000000	-3.4100551
H	4.7073598	0.0000000	-1.3630236
H	4.7073598	0.0000000	1.3630236
H	3.4411050	0.0000000	3.4100551
H	1.2161081	0.0000000	4.7060517
H	-1.2161081	0.0000000	4.7060517
Li	0.0000000	1.6308646	0.0000000
Li	0.0000000	-1.6308646	0.0000000
H	1.265355989	-3.378466779	0.000000000
H	1.755650811	-2.821533221	0.000000000
H	-1.265355989	3.378466779	0.000000000
H	-1.755650811	2.821533221	0.000000000

CoroB₂Li₂...H₂ss

B	-1.2352545	-0.7589914	0.2440153
C	0.0835516	-1.5055002	0.2068561
C	1.2999472	-0.7639774	0.2181541
B	1.2352545	0.7589914	0.2440153
C	-0.0835516	1.5055002	0.2068561
C	-1.2999472	0.7639774	0.2181541
C	-2.5621581	1.4310699	0.2237340
C	-3.7604463	0.6197511	0.2268484
C	-3.7476387	-0.7856602	0.2354274
C	-2.5287787	-1.5429666	0.2126965
C	-2.4085636	-2.9776999	0.1972006
C	-1.1796036	-3.6107921	0.1935893
C	0.0857498	-2.9163067	0.1974978
C	1.3589737	-3.5708701	0.1988809
C	2.5461200	-2.8647988	0.2094780
C	2.5621581	-1.4310699	0.2237340
C	3.7604463	-0.6197511	0.2268484
C	3.7476387	0.7856602	0.2354274
C	2.5287787	1.5429666	0.2126965
C	2.4085636	2.9776999	0.1972006
C	1.1796036	3.6107921	0.1935893
C	-0.0857498	2.9163067	0.1974978
C	-1.3589737	3.5708701	0.1988809
C	-2.5461200	2.8647988	0.2094780
H	-4.7241842	1.1227568	0.2369714
H	-4.7156902	-1.2884340	0.2460590
H	-3.3012306	-3.6041263	0.2058115
H	-1.1627405	-4.6984490	0.1935973
H	1.3998458	-4.6578941	0.1977927
H	3.4865623	-3.4109225	0.2199907
H	4.7241842	-1.1227568	0.2369714
H	4.7156902	1.2884340	0.2460590
H	3.3012306	3.6041263	0.2058115
H	1.1627405	4.6984490	0.1935973
H	-1.3998458	4.6578941	0.1977927
H	-3.4865623	3.4109225	0.2199907
Li	2.5371572	0.0550250	-1.4251734
Li	-2.5371572	-0.0550250	-1.4251734
H	0.0000000	0.0000000	-2.3965165
H	0.0000000	0.0000000	-3.1385165

CoroB₂Li₂...H₂os

B	-1.2346188	-0.7591096	-0.0252158
C	0.0838219	-1.5047497	-0.0699789
C	1.2996830	-0.7634572	-0.0476769
B	1.2346188	0.7591096	-0.0252158
C	-0.0838219	1.5047497	-0.0699789
C	-1.2996830	0.7634572	-0.0476769
C	-2.5616433	1.4310103	-0.0465761
C	-3.7600980	0.6202450	-0.0469607
C	-3.7471284	-0.7848341	-0.0449410
C	-2.5281870	-1.5416302	-0.0667751
C	-2.4084166	-2.9754876	-0.1045707
C	-1.1799761	-3.6091762	-0.1128425
C	0.0856989	-2.9151894	-0.0956446
C	1.3587281	-3.5699447	-0.1012857
C	2.5456375	-2.8637667	-0.0799923
C	2.5616433	-1.4310103	-0.0465761
C	3.7600980	-0.6202450	-0.0469607
C	3.7471284	0.7848341	-0.0449410
C	2.5281870	1.5416302	-0.0667751
C	2.4084166	2.9754876	-0.1045707
C	1.1799761	3.6091762	-0.1128425
C	-0.0856989	2.9151894	-0.0956446
C	-1.3587281	3.5699447	-0.1012857
C	-2.5456375	2.8637667	-0.0799923
H	-4.7232960	1.1228692	-0.0497581
H	-4.7143959	-1.2873366	-0.0507759
H	-3.3013141	-3.6015506	-0.1088096
H	-1.1636195	-4.6967228	-0.1291146
H	1.3994879	-4.6568924	-0.1172680
H	3.4860882	-3.4099578	-0.0760191
H	4.7232960	-1.1228692	-0.0497581
H	4.7143959	1.2873366	-0.0507759
H	3.3013141	3.6015506	-0.1088096
H	1.1636195	4.6967228	-0.1291146
H	-1.3994879	4.6568924	-0.1172680
H	-3.4860882	3.4099578	-0.0760191
Li	2.5289649	0.0431623	-1.6715860
Li	-2.5289649	-0.0431623	-1.6715860
H	0.0000000	0.0000000	2.7327751
H	0.0000000	0.0000000	3.4747751