Supplementary Material

Table S1. Cartesian coordinates (in Å) for the optimized structures of isolated species and $Li_6(H_2)_n$ complexes at the wB97X-D4rev/def2-TZVPPD level of theory.

System	Isomer		x	y	z
H_2	-	H	0.87146964	0.00000000	0.00000000
H_2	-	H	0.12853036	0.00000000	0.00000000
Li_6	-	Li	0.70935177	0.69794262	0.29287608
Li_6	-	Li	0.54051366	2.95908903	-1.40080409
Li_6	-	Li	0.35155161	2.92334991	1.42279662
Li_6	-	Li	0.52047637	0.66220829	3.11647855
Li_6	-	Li	3.03867200	2.12670638	1.02953714
Li_6	-	Li	-1.97776736	1.49468121	0.68592539
$Li_6(H_2)_1$	0	Li	0.71478173	0.66411795	0.27561742
$Li_6(H_2)_1$	0	Li	0.51965800	2.96846520	-1.38440702
$Li_6(H_2)_1$	0	Li	0.35667483	2.89149959	1.40657936
$Li_6(H_2)_1$	0	Li	0.53608895	0.68570455	3.11665598
$Li_6(H_2)_1$	0	Li	3.02551409	2.13346576	1.05365836
$Li_6(H_2)_1$	0	Li	-1.96991955	1.52072440	0.67870560
$Li_6(H_2)_1$	0	H	-0.18678666	4.45919486	2.49962313
$Li_6(H_2)_1$	0	H	0.34574911	4.76709776	2.06222133
$Li_6(H_2)_2$	1	Li	0.28227865	0.68683728	0.25679241
$Li_6(H_2)_2$	1	Li	0.43087269	2.84611726	-1.55752380
$Li_6(H_2)_2$	1	Li	0.52896947	2.97458528	1.26206373
$Li_6(H_2)_2$	1	Li	0.17610703	0.83795012	3.07499899
$Li_6(H_2)_2$	1	Li	2.94862676	1.54873945	0.77699646
$Li_6(H_2)_2$	1	Li	-2.11845636	2.11060035	0.74195642
$Li_6(H_2)_2$	1	H	-4.58632780	2.53498122	0.38213575
$Li_6(H_2)_2$	1	H	-4.62424454	2.23863367	1.06599700
$Li_6(H_2)_2$	0	Li	0.71970833	0.57437234	0.21574308

$Li_6(H_2)_2$	0	Li	0.62446897	2.78460037	-1.52531647
$Li_6(H_2)_2$	0	Li	0.49079346	2.86500453	1.28557680
$Li_6(H_2)_2$	0	Li	0.58572675	0.65469189	3.02658796
$Li_6(H_2)_2$	0	Li	3.10786249	1.91672139	0.86410845
$Li_6(H_2)_2$	0	Li	-1.89735941	1.52268128	0.63711430
$Li_6(H_2)_2$	0	H	0.04565019	4.51371107	2.34754384
$Li_6(H_2)_2$	0	H	0.57961556	4.78150770	1.88831502
$Li_6(H_2)_2$	0	H	1.16009993	-1.30015506	-0.36433723
$Li_6(H_2)_2$	0	H	0.63380785	-1.11553394	-0.87094743
$Li_6(H_2)_2$	1	Li	0.50915425	0.52665429	0.48987899
$Li_6(H_2)_2$	1	Li	0.47670233	2.44845744	-1.54245598
$Li_6(H_2)_2$	1	Li	0.57147789	2.92816818	1.26121676
$Li_6(H_2)_2$	1	Li	0.60108857	0.90142536	3.26087182
$Li_6(H_2)_2$	1	Li	3.06255614	1.62213492	0.81827293
$Li_6(H_2)_2$	1	Li	-1.98365605	1.72821892	0.90037367
$Li_6(H_2)_2$	1	H	0.71143334	-1.24796698	-0.37505757
$Li_6(H_2)_2$	1	H	0.18911898	-1.40170793	0.14709727
$Li_6(H_2)_2$	1	H	-1.69066691	-1.82071321	-2.39896676
$Li_6(H_2)_2$	1	H	-1.59650586	-1.14210882	-2.10780376
$Li_6(H_2)_2$	2	Li	0.51520991	0.46903928	0.21623800
$Li_6(H_2)_2$	2	Li	0.38164649	2.94397170	-1.16869487
$Li_6(H_2)_2$	2	Li	0.77291464	2.57305128	1.56884005
$Li_6(H_2)_2$	2	Li	0.76547252	0.19231108	3.03111379
$Li_6(H_2)_2$	2	Li	3.16793471	1.48290784	0.57622001
$Li_6(H_2)_2$	2	Li	-1.85630764	1.66723383	1.24749526
$Li_6(H_2)_2$	2	H	0.65328818	4.34706217	2.45286502
$Li_6(H_2)_2$	2	H	1.29320579	4.08220199	2.75246908
$Li_6(H_2)_2$	2	H	-4.36878267	1.52573725	1.84296472
$Li_6(H_2)_2$	2	H	-4.42673244	1.95020084	1.23252392
$Li_6(H_2)_2$	3	Li	1.25274030	0.14349429	0.13129316
$Li_6(H_2)_2$	3	Li	-1.25440065	-0.10895968	-0.03894584

$Li_6(H_2)_2$	3	Li	-0.21749086	2.52195980	0.27086169
$Li_6(H_2)_2$	3	Li	0.31399495	-2.47942789	-0.16583457
$Li_6(H_2)_2$	3	Li	-0.10249581	-0.18305797	2.56153410
$Li_6(H_2)_2$	3	Li	0.19978337	0.22140967	-2.46162413
$Li_6(H_2)_2$	3	H	3.20085190	0.04008412	0.51741313
$Li_6(H_2)_2$	3	H	3.19008063	0.61507960	0.02996109
$Li_6(H_2)_2$	3	H	4.59857388	2.63550338	-1.45528751
$Li_6(H_2)_2$	3	H	3.86076411	2.61404898	-1.55034223
$Li_6(H_2)_2$					
$Li_6(H_2)_2$	4	Li	1.15871158	0.89403695	0.32369566
$Li_6(H_2)_2$	4	Li	1.07251433	3.43031010	-0.91574130
$Li_6(H_2)_2$	4	Li	0.23916336	2.76802395	1.70255703
$Li_6(H_2)_2$	4	Li	0.70643723	0.33425623	3.05702456
$Li_6(H_2)_2$	4	Li	3.06636672	2.46765723	1.72731714
$Li_6(H_2)_2$	4	Li	-1.69750075	1.18734038	0.29048541
$Li_6(H_2)_2$	4	H	4.12034773	3.61959260	3.58182614
$Li_6(H_2)_2$	4	H	4.58785296	3.94823137	3.10101099
$Li_6(H_2)_2$	4	H	5.32938654	2.25993713	0.92742342
$Li_6(H_2)_2$	4	H	5.54068509	2.10185492	1.62613706
$Li_6(H_2)_2$					
$Li_6(H_2)_2$	5	Li	0.63855673	0.56714281	0.25362921
$Li_6(H_2)_2$	5	Li	0.65884273	2.72229751	-1.56165056
$Li_6(H_2)_2$	5	Li	0.53033543	2.86588660	1.24961277
$Li_6(H_2)_2$	5	Li	0.51028326	0.71075268	3.06491073
$Li_6(H_2)_2$	5	Li	3.13254730	1.78766063	0.86433622
$Li_6(H_2)_2$	5	Li	-1.96367649	1.64543545	0.63883962
$Li_6(H_2)_2$	5	H	5.95697051	2.01275116	0.65077043
$Li_6(H_2)_2$	5	H	5.93321471	1.71529825	1.33336345
$Li_6(H_2)_2$	5	H	-4.76688703	1.71705379	0.17147094
$Li_6(H_2)_2$	5	H	-4.78969482	1.41983134	0.85418777
$Li_6(H_2)_3$	0	Li	1.21972943	0.06869328	0.08193308
$Li_6(H_2)_3$	0	Li	-1.31285765	-0.04433116	-0.05754191
$Li_6(H_2)_3$	0	Li	-0.15655409	2.52225571	-0.01378847

$Li_6(H_2)_3$	0	Li	0.06480764	-2.49868569	0.04238432
$Li_6(H_2)_3$	0	Li	-0.18533477	0.03996154	2.52084724
$Li_6(H_2)_3$	0	Li	0.09371841	-0.01142582	-2.49730598
$Li_6(H_2)_3$	0	H	3.18335011	-0.09588943	0.47028377
$Li_6(H_2)_3$	0	H	3.18951693	0.43093726	-0.06801119
$Li_6(H_2)_3$	0	H	-3.31027948	0.14152792	0.10146284
$Li_6(H_2)_3$	0	H	-3.26015321	-0.39602997	-0.42386249
$Li_6(H_2)_3$	0	H	4.14549068	2.33217483	2.32831377
$Li_6(H_2)_3$	0	H	3.41622157	2.23014681	2.22070956
$Li_6(H_2)_3$	1	Li	1.13455408	0.20544752	-0.06473554
$Li_6(H_2)_3$	1	Li	-1.38981028	0.05760460	0.04031899
$Li_6(H_2)_3$	1	Li	-0.24674693	2.58041165	0.51240663
$Li_6(H_2)_3$	1	Li	-0.01446262	-2.29224888	-0.64393777
$Li_6(H_2)_3$	1	Li	0.00834534	-0.44551894	2.44658290
$Li_6(H_2)_3$	1	Li	-0.26324398	0.70626091	-2.46101199
$Li_6(H_2)_3$	1	H	3.13378033	0.02092302	0.06924018
$Li_6(H_2)_3$	1	H	3.07608388	0.64174423	-0.35362443
$Li_6(H_2)_3$	1	H	-3.35877150	0.11356949	0.45090772
$Li_6(H_2)_3$	1	H	-3.36106990	-0.25181625	-0.20788727
$Li_6(H_2)_3$	1	H	-0.40483769	1.67725233	-4.95854001
$Li_6(H_2)_3$	1	H	-0.41011713	0.95182044	-5.12919794
$Li_6(H_2)_3$	2	Li	1.18320653	-0.01998500	0.07807145
$Li_6(H_2)_3$	2	Li	-1.32841653	0.03175965	-0.17244440
$Li_6(H_2)_3$	2	Li	0.02659496	2.52792366	-0.01234683
$Li_6(H_2)_3$	2	Li	-0.06801653	-2.51787414	-0.06386809
$Li_6(H_2)_3$	2	Li	-0.27592952	0.02326944	2.46951631
$Li_6(H_2)_3$	2	Li	0.22254036	-0.00344261	-2.55685595
$Li_6(H_2)_3$	2	H	3.10885963	-0.32307531	0.49720394
$Li_6(H_2)_3$	2	H	3.14890245	0.26256742	0.02452040
$Li_6(H_2)_3$	2	H	4.09959344	1.54277098	2.87175545
$Li_6(H_2)_3$	2	H	3.39893815	1.59912169	2.62742182
$Li_6(H_2)_3$	2	H	3.54739959	-1.62232284	2.77885190

$Li_6(H_2)_3$	2	H	4.26928546	-1.49756511	2.90882621
$Li_6(H_2)_3$	3	Li	1.12608805	0.19263705	0.78538442
$Li_6(H_2)_3$	3	Li	-1.33485558	0.77830237	-0.51849984
$Li_6(H_2)_3$	3	Li	0.32081102	2.58306628	0.83467588
$Li_6(H_2)_3$	3	Li	2.74770239	2.09837293	2.14082854
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$Li_6(H_2)_3$	4	Li	0.69588348	0.43310422	0.39642440
$Li_6(H_2)_3$	4	Li	0.81127915	2.53992921	-1.53544867
$Li_6(H_2)_3$	4	Li	0.60123873	2.79333243	1.25718074
$Li_6(H_2)_3$	4	Li	0.45249483	0.79619880	3.21364615
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$Li_6(H_2)_3$	4	Li	-1.86475342	1.62485549	0.67598061
$Li_6(H_2)_3$	4	H	0.62923119	-0.15569178	5.64184720
$Li_6(H_2)_3$	4	H	-0.11438450	-0.14028297	5.59077660
$Li_6(H_2)_3$	4	H	-1.64591527	6.42217069	0.34779428
$Li_6(H_2)_3$	4	H	-1.49026461	5.72435949	0.14082732
$Li_6(H_2)_3$	4	H	0.76045089	4.73171018	1.65150250
$Li_6(H_2)_3$	4	H	0.24847805	4.52166741	2.16418198
$Li_6(H_2)_3$	5	Li	0.70224982	0.61302791	0.25757517
$Li_6(H_2)_3$	5	Li	0.50441304	2.84482052	-1.51740992
$Li_6(H_2)_3$	5	Li	0.49286246	2.89278608	1.28993751
$Li_6(H_2)_3$	5	Li	0.68122087	0.76459015	3.11163908
$Li_6(H_2)_3$	5	Li	3.09585168	2.04142977	0.76979222
$Li_6(H_2)_3$	5	Li	-1.90936733	1.55828086	0.82145061

$Li_6(H_2)_3$	5	H	1.19023771	-0.41004094	5.69321816
$Li_6(H_2)_3$	5	H	0.45145192	-0.50384313	5.68893910
$Li_6(H_2)_3$	5	H	0.74782068	3.98739775	-4.16220210
$Li_6(H_2)_3$	5	H	0.00473688	3.94110763	-4.14592449
$Li_6(H_2)_3$	5	H	0.10753857	4.77104519	1.80698877
$Li_6(H_2)_3$	5	H	0.55247053	4.55397425	2.37639530
$Li_6(H_2)_3$	6	Li	0.59903655	0.57875018	0.23351461
$Li_6(H_2)_3$	6	Li	1.31448776	2.77643603	-1.40731613
$Li_6(H_2)_3$	6	Li	0.51455897	2.83652115	1.31125479
$Li_6(H_2)_3$	6	Li	-0.35187303	0.65685694	2.90244864
$Li_6(H_2)_3$	6	Li	2.96061278	1.42097086	1.56128182
$Li_6(H_2)_3$	6	Li	-1.82962609	1.99193736	-0.01023705
$Li_6(H_2)_3$	6	H	-0.70785068	-0.64574293	5.59641899
$Li_6(H_2)_3$	6	H	-1.43754527	-0.60490711	5.45485474
$Li_6(H_2)_3$	6	H	2.89096636	3.93358157	-3.70332541
$Li_6(H_2)_3$	6	H	2.22884962	4.05883451	-4.01960629
$Li_6(H_2)_3$	6	H	-4.27281364	2.45259303	-1.16624212
$Li_6(H_2)_3$	6	H	-4.51646280	2.14226738	-0.53415146
$Li_6(H_2)_4$	0	Li	0.91039519	0.43983405	0.63167578
$Li_6(H_2)_4$	0	Li	0.41645511	2.51292700	-1.20689549
$Li_6(H_2)_4$	0	Li	0.20493186	2.68098984	1.59469855
$Li_6(H_2)_4$	0	Li	0.69854568	0.60726341	3.43501190
$Li_6(H_2)_4$	0	Li	2.96718648	2.26070658	1.24985279
$Li_6(H_2)_4$	0	Li	-1.85225376	0.86305243	0.96902242
$Li_6(H_2)_4$	0	H	-0.59173856	4.25321285	2.55989180
$Li_6(H_2)_4$	0	H	-0.11203449	4.60118468	2.09513540
$Li_6(H_2)_4$	0	H	1.73552827	-1.32210800	0.12860581
$Li_6(H_2)_4$	0	H	1.19300483	-1.26685784	-0.39082683
$Li_6(H_2)_4$	0	H	-2.55580034	5.00736004	0.52118880
$Li_6(H_2)_4$	0	H	-2.83464728	5.66476624	0.73041921
$Li_6(H_2)_4$	0	H	3.42245419	-0.34373526	-2.05898421
$Li_6(H_2)_4$	0	H	3.68815636	-0.94637046	-2.40532229

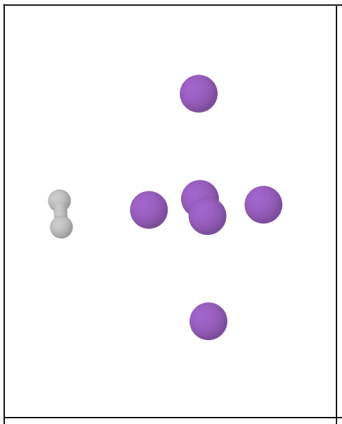
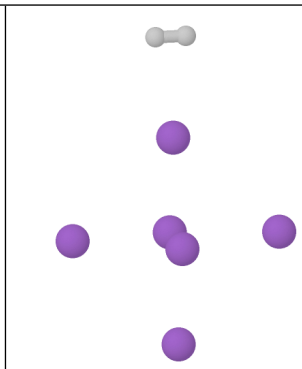
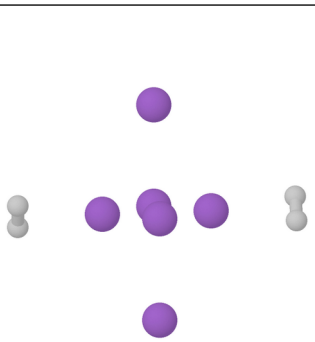
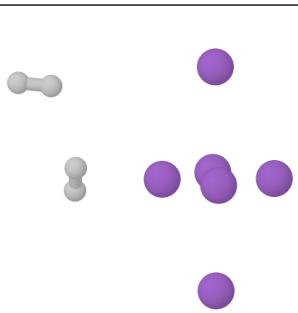
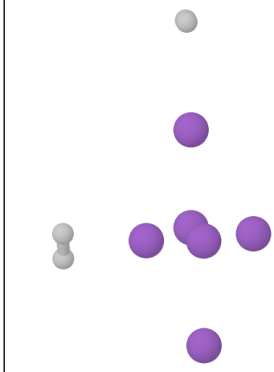
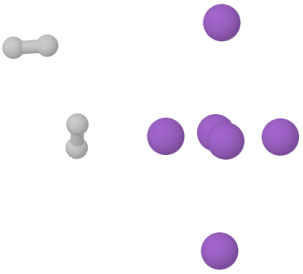
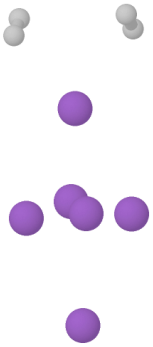
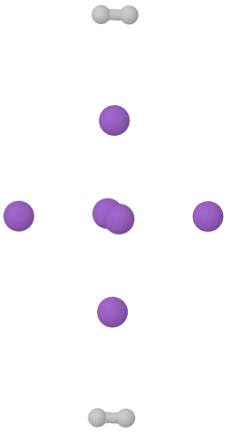
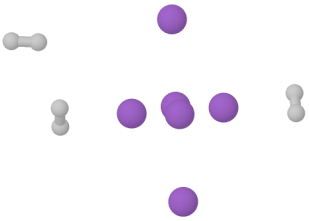
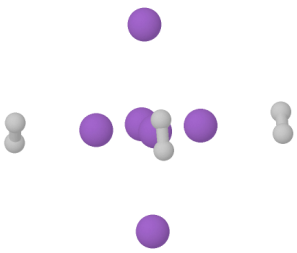
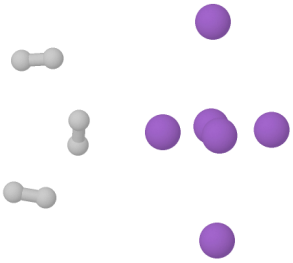
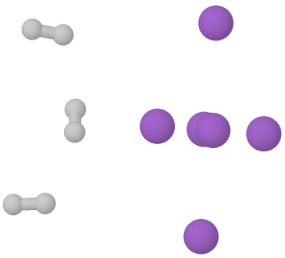
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$Li_6(H_2)_4$	1	Li	0.81262853	2.52414422	-1.53677673
$Li_6(H_2)_4$	1	Li	0.13559153	2.93585953	1.16883172
$Li_6(H_2)_4$	1	Li	0.30392284	1.01985968	3.23142132
$Li_6(H_2)_4$	1	Li	2.90651333	2.50551934	1.35368953
$Li_6(H_2)_4$	1	Li	-1.80956936	1.08260892	0.34266277
$Li_6(H_2)_4$	1	H	-2.14470730	5.31051201	-0.69607753
$Li_6(H_2)_4$	1	H	-2.37212107	6.01605235	-0.63105739
$Li_6(H_2)_4$	1	H	3.78514049	-1.51965341	1.99548574
$Li_6(H_2)_4$	1	H	4.12592565	-2.15422968	1.80856249
$Li_6(H_2)_4$	1	H	-0.19172439	4.87613719	1.59123112
$Li_6(H_2)_4$	1	H	-0.86805713	4.58137757	1.74202553
$Li_6(H_2)_4$	1	H	1.65451292	-1.07118690	-0.32299054
$Li_6(H_2)_4$	1	H	1.57043042	-1.29761954	0.39002168
$Li_6(H_2)_4$					
$Li_6(H_2)_4$	2	Li	1.15433471	0.98779154	0.46183421
$Li_6(H_2)_4$	2	Li	0.24087023	3.09428424	-1.15302727
$Li_6(H_2)_4$	2	Li	0.81435241	3.22603238	1.59394039
$Li_6(H_2)_4$	2	Li	1.63278362	1.09371760	3.22878054
$Li_6(H_2)_4$	2	Li	3.38654719	2.72045923	0.53494559
$Li_6(H_2)_4$	2	Li	-1.41179337	1.49699409	1.51047051
$Li_6(H_2)_4$	2	H	0.36461542	4.80362362	2.75878847
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$Li_6(H_2)_4$	2	H	1.76209169	-0.77898391	-0.27670680
$Li_6(H_2)_4$	2	H	1.09119794	-0.70800901	-0.61167093
$Li_6(H_2)_4$	2	H	-3.86715584	0.71926234	2.38164730
$Li_6(H_2)_4$	2	H	-4.07441453	0.97371660	1.71274238
$Li_6(H_2)_4$	2	H	2.77507057	0.18964825	-2.84760845
$Li_6(H_2)_4$	2	H	2.89444902	-0.40529129	-3.27839138
$Li_6(H_2)_4$	3	Li	0.76602341	-0.25566559	0.04816335
$Li_6(H_2)_4$	3	Li	0.51127621	1.89480535	-1.74539546
$Li_6(H_2)_4$	3	Li	0.40401294	2.04397182	1.06962397

$Li_6(H_2)_4$	3	Li	0.66171404	-0.12471017	2.85510552
$Li_6(H_2)_4$	3	Li	3.07276699	1.24544921	0.62496970
$Li_6(H_2)_4$	3	Li	-1.89985693	0.52449952	0.48511285
$Li_6(H_2)_4$	3	H	-0.13558843	3.69522220	2.10340114
$Li_6(H_2)_4$	3	H	0.37579418	3.98501697	1.63379958
$Li_6(H_2)_4$	3	H	1.32003450	-2.11189754	-0.49187993
$Li_6(H_2)_4$	3	H	0.77780625	-1.97409879	-0.99630146
$Li_6(H_2)_4$	3	H	2.03227711	5.60904271	0.29951603
$Li_6(H_2)_4$	3	H	1.89090102	6.25905388	0.63272754
$Li_6(H_2)_4$	3	H	-1.98198710	3.33939343	4.00668635
$Li_6(H_2)_4$	3	H	-2.04870390	4.03215625	4.26966234
$Li_6(H_2)_4$	4	Li	0.59634109	0.39124772	0.60593981
$Li_6(H_2)_4$	4	Li	0.51945565	2.57667740	-1.16721291
$Li_6(H_2)_4$	4	Li	0.58230748	2.71206179	1.64399754
$Li_6(H_2)_4$	4	Li	0.65967783	0.52580326	3.41996876
$Li_6(H_2)_4$	4	Li	3.10177888	1.59288370	1.07127881
$Li_6(H_2)_4$	4	Li	-1.92292599	1.50708546	1.18634201
$Li_6(H_2)_4$	4	H	0.29728945	4.39785373	2.70549503
$Li_6(H_2)_4$	4	H	0.81660422	4.63595818	2.21529184
$Li_6(H_2)_4$	4	H	0.89661149	-1.51725818	0.04268577
$Li_6(H_2)_4$	4	H	0.34768364	-1.32310217	-0.43443920
$Li_6(H_2)_4$	4	H	-1.49667632	-1.98362423	-2.58502108
$Li_6(H_2)_4$	4	H	-1.54101707	-1.28902784	-2.32209982
$Li_6(H_2)_4$	4	H	2.61951577	6.05648303	0.84439251
$Li_6(H_2)_4$	4	H	2.58169253	6.71470322	1.18917122
$Li_6(H_2)_4$	5	Li	0.49559554	0.78116869	0.26087936
$Li_6(H_2)_4$	5	Li	0.78795187	2.74452336	-1.73058666
$Li_6(H_2)_4$	5	Li	0.37157294	3.19760138	1.00986640
$Li_6(H_2)_4$	5	Li	0.18586767	1.24501641	3.01631388
$Li_6(H_2)_4$	5	Li	2.93217395	2.02346302	0.95878212
$Li_6(H_2)_4$	5	Li	-2.07343738	1.96476456	0.31285191
$Li_6(H_2)_4$	5	H	5.56793206	1.96980807	1.65970366

$Li_6(H_2)_4$	5	H	5.65594820	2.15820226	0.94424920
$Li_6(H_2)_4$	5	H	-1.56541584	-3.17182112	0.94280266
$Li_6(H_2)_4$	5	H	-1.65094861	-2.47226996	1.18127977
$Li_6(H_2)_4$	5	H	0.02209961	5.15287778	1.33168041
$Li_6(H_2)_4$	5	H	0.51388979	5.00354689	1.88241690
$Li_6(H_2)_4$	5	H	0.90860675	-1.01516694	-0.54659849
$Li_6(H_2)_4$	5	H	0.29983686	-1.19053566	-0.13991328
$Li_6(H_2)_4$	6	Li	-0.61874119	1.18887963	0.53425987
$Li_6(H_2)_4$	6	Li	0.23090060	2.92454634	-1.57287027
$Li_6(H_2)_4$	6	Li	1.50899974	2.47449053	0.88599888
$Li_6(H_2)_4$	6	Li	0.75527981	0.79803829	3.00766239
$Li_6(H_2)_4$	6	Li	1.80257608	-0.04443825	-0.26967736
$Li_6(H_2)_4$	6	Li	-0.82288630	3.75999541	1.71011907
$Li_6(H_2)_4$	6	H	1.20207281	-0.69159087	5.47281271
$Li_6(H_2)_4$	6	H	0.84638373	-0.11196960	5.77599622
$Li_6(H_2)_4$	6	H	5.53064404	1.63163305	2.43937448
$Li_6(H_2)_4$	6	H	4.85475415	1.36766108	2.27382609
$Li_6(H_2)_4$	6	H	3.25503926	3.41423267	0.81312033
$Li_6(H_2)_4$	6	H	3.06974954	3.50969340	1.53813142
$Li_6(H_2)_4$	6	H	-0.31723506	4.36399816	-4.06415846
$Li_6(H_2)_4$	6	H	0.09402402	3.81926093	-4.36162399
$Li_6(H_2)_4$	7	Li	0.84958727	0.48460875	0.07105222
$Li_6(H_2)_4$	7	Li	0.68679423	2.57970079	-1.76409244
$Li_6(H_2)_4$	7	Li	0.65226279	2.77849687	1.06620933
$Li_6(H_2)_4$	7	Li	0.84701417	0.58359223	2.87113782
$Li_6(H_2)_4$	7	Li	3.27587955	1.80059243	0.53914466
$Li_6(H_2)_4$	7	Li	-1.76954365	1.40624647	0.45626466
$Li_6(H_2)_4$	7	H	1.28613928	-1.16987382	-0.93791870
$Li_6(H_2)_4$	7	H	0.74412580	-1.42323249	-0.47840860
$Li_6(H_2)_4$	7	H	1.00139914	3.72591673	-4.36990879
$Li_6(H_2)_4$	7	H	0.25760348	3.68908438	-4.36986949
$Li_6(H_2)_4$	7	H	6.31117694	2.15129183	0.39781833

$Li_6(H_2)_4$	7	H	6.26270863	1.87103790	1.08564394
$Li_6(H_2)_4$	7	H	-4.87383568	1.23471868	0.33130622
$Li_6(H_2)_4$	7	H	-4.76423223	0.91362452	0.99367023
$Li_6(H_2)_4$	8	Li	0.70267714	0.57806162	0.22557783
$Li_6(H_2)_4$	8	Li	0.65296461	2.74189953	-1.59738659
$Li_6(H_2)_4$	8	Li	0.47131005	2.86190245	1.22401102
$Li_6(H_2)_4$	8	Li	0.52158158	0.69808573	3.04700613
$Li_6(H_2)_4$	8	Li	3.11316070	1.90842297	0.87909894
$Li_6(H_2)_4$	8	Li	-1.93919209	1.53164850	0.57025051
$Li_6(H_2)_4$	8	H	0.80912494	-0.52350444	5.90003562
$Li_6(H_2)_4$	8	H	0.06845653	-0.57857855	5.85311229
$Li_6(H_2)_4$	8	H	-5.01290073	1.44938603	0.04235444
$Li_6(H_2)_4$	8	H	-5.03128878	1.15009084	0.72345468
$Li_6(H_2)_4$	8	H	6.18439535	1.99029704	1.40990071
$Li_6(H_2)_4$	8	H	6.20415149	2.28937911	0.72873796
$Li_6(H_2)_4$	8	H	0.36169839	3.96289240	-4.44973402
$Li_6(H_2)_4$	8	H	1.10246368	4.01817993	-4.40467797

Figure S1. Optimized geometries for all studied $Li_6(H_2)_n$ (n=1–4) isomers at the wB97X-D4rev/def2-TZVPPD level of theory. Structural labels correspond to the Cartesian coordinates provided in Table S1.

			
Li6(H2)1_iso_0 (GM)	Li6(H2)1_iso_1	Li6(H2)2_iso_0 (GM)	Li6(H2)2_iso_1
			
Li6(H2)2_iso_2	Li6(H2)2_iso_3	Li6(H2)2_iso_4	Li6(H2)2_iso_5
			
Li6(H2)3_iso_0 (GM)	Li6(H2)3_iso_1	Li6(H2)3_iso_2	Li6(H2)3_iso_3

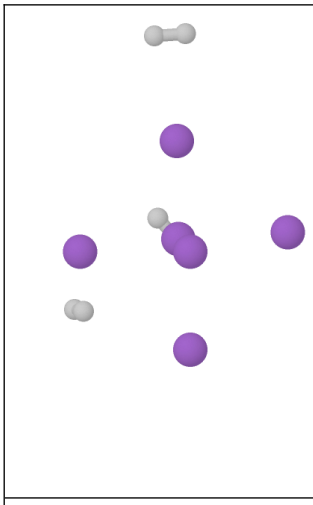
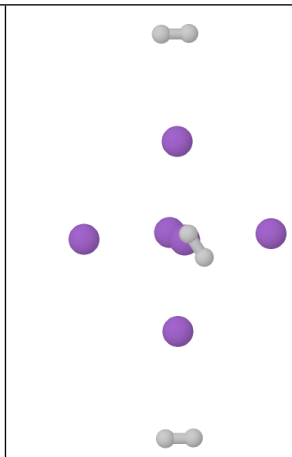
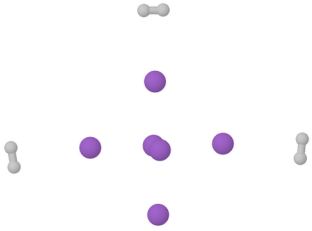
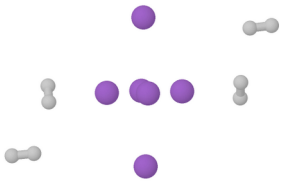
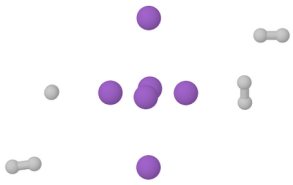
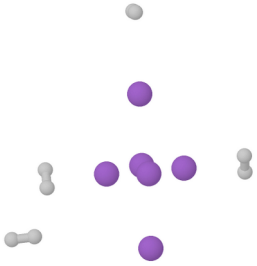
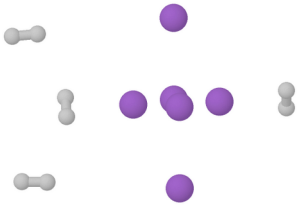
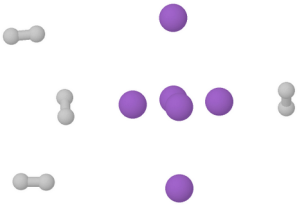
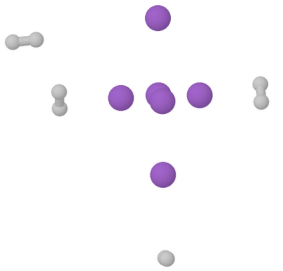
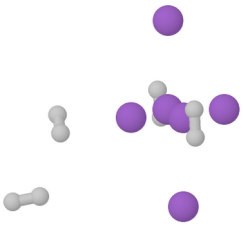
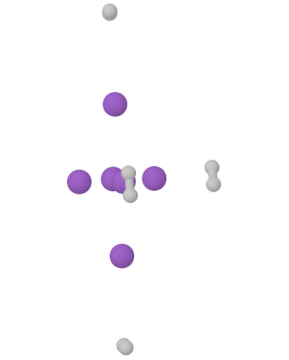
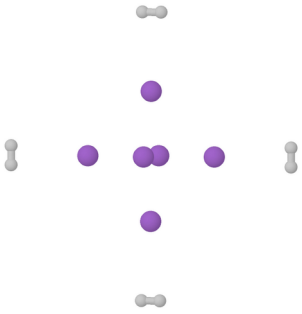
			
Li6(H2)3_iso_4	Li6(H2)3_iso_5	Li6(H2)3_iso_6	Li6(H2)4_iso_0
			
Li6(H2)4_iso_1 (GM)	Li6(H2)4_iso_2	Li6(H2)4_iso_3	Li6(H2)4_iso_4
			
Li6(H2)4_iso_5	Li6(H2)4_iso_6	Li6(H2)4_iso_7	Li6(H2)4_iso_8

Table S2. Total electronic energies and counterpoise components (CP) at the wB97X-D4rev/def2-TZVPPD level of theory. All values are reported in atomic units (a.u.).

System	Isomer	Calculation Component	Electronic Energy
$Li_6(H_2)_1$	0	$Li_6(H_2)_1$ (Complex)	-46.315568786927
$Li_6(H_2)_1$	0	Li_6 (in complex)	-45.126523723035
$Li_6(H_2)_1$	0	H_2 (in complex)	-1.181718882771
$Li_6(H_2)_1$	0	Li_6 (ghost)	-45.126941899804
$Li_6(H_2)_1$	0	H_2 (ghost)	-1.181710650102
$Li_6(H_2)_1$	1	$Li_6(H_2)_1$ (Complex)	-46.30956118807
$Li_6(H_2)_1$	1	Li_6 (in complex)	-45.126566655784
$Li_6(H_2)_1$	1	H_2 (in complex)	-1.181803533918
$Li_6(H_2)_1$	1	Li_6 (ghost)	-45.126665279982
$Li_6(H_2)_1$	1	H_2 (ghost)	-1.181804384969
$Li_6(H_2)_2$	0	$Li_6(H_2)_2$ (Complex)	-47.503418481363
$Li_6(H_2)_2$	0	Li_6 (in complex)	-45.126582478014
$Li_6(H_2)_2$	0	$2H_2$ (in complex)	-2.363478552211
$Li_6(H_2)_2$	0	Li_6 (ghost)	-45.127303509186
$Li_6(H_2)_2$	0	$2H_2$ (ghost)	-2.363463376804
$Li_6(H_2)_2$	1	$Li_6(H_2)_2$ (Complex)	-47.498407160939
$Li_6(H_2)_2$	1	Li_6 (in complex)	-45.126526277706
$Li_6(H_2)_2$	1	$2H_2$ (in complex)	-2.363569854689
$Li_6(H_2)_2$	1	Li_6 (ghost)	-45.127109866194
$Li_6(H_2)_2$	1	$2H_2$ (ghost)	-2.363560610093
$Li_6(H_2)_2$	2	$Li_6(H_2)_2$ (Complex)	-47.498042884822
$Li_6(H_2)_2$	2	Li_6 (in complex)	-45.126491731133
$Li_6(H_2)_2$	2	$2H_2$ (in complex)	-2.363534538595
$Li_6(H_2)_2$	2	Li_6 (ghost)	-45.126976187016
$Li_6(H_2)_2$	2	$2H_2$ (ghost)	-2.363525923165

$Li_6(H_2)_2$	3	$Li_6(H_2)_2$ (Complex)	-47.498199721708
$Li_6(H_2)_2$	3	Li_6 (in complex)	-45.126546314602
$Li_6(H_2)_2$	3	$2H_2$ (in complex)	-2.363645989572
$Li_6(H_2)_2$	3	Li_6 (ghost)	-45.127031005966
$Li_6(H_2)_2$	3	$2H_2$ (ghost)	-2.363633519507
$Li_6(H_2)_2$	4	$Li_6(H_2)_2$ (Complex)	-47.492684522668
$Li_6(H_2)_2$	4	Li_6 (in complex)	-45.126374198113
$Li_6(H_2)_2$	4	$2H_2$ (in complex)	-2.363449617964
$Li_6(H_2)_2$	4	Li_6 (ghost)	-45.126600377917
$Li_6(H_2)_2$	4	$2H_2$ (ghost)	-2.363446987588
$Li_6(H_2)_2$	5	$Li_6(H_2)_2$ (Complex)	-47.49187028126
$Li_6(H_2)_2$	5	Li_6 (in complex)	-45.126599230811
$Li_6(H_2)_2$	5	$2H_2$ (in complex)	-2.363616444744
$Li_6(H_2)_2$	5	Li_6 (ghost)	-45.126727154504
$Li_6(H_2)_2$	5	$2H_2$ (ghost)	-2.363622562566
$Li_6(H_2)_3$	0	$Li_6(H_2)_3$ (Complex)	-48.686058568666
$Li_6(H_2)_3$	0	Li_6 (in complex)	-45.126581310417
$Li_6(H_2)_3$	0	$3H_2$ (in complex)	-3.545345849558
$Li_6(H_2)_3$	0	Li_6 (ghost)	-45.127446691977
$Li_6(H_2)_3$	0	$3H_2$ (ghost)	-3.545331172433
$Li_6(H_2)_3$	1	$Li_6(H_2)_3$ (Complex)	-48.685648815496
$Li_6(H_2)_3$	1	Li_6 (in complex)	-45.12656675687
$Li_6(H_2)_3$	1	$3H_2$ (in complex)	-3.545300217412
$Li_6(H_2)_3$	1	Li_6 (ghost)	-45.127344844846
$Li_6(H_2)_3$	1	$3H_2$ (ghost)	-3.545285722546
$Li_6(H_2)_3$	2	$Li_6(H_2)_3$ (Complex)	-48.68117165347
$Li_6(H_2)_3$	2	Li_6 (in complex)	-45.12654567223
$Li_6(H_2)_3$	2	$3H_2$ (in complex)	-3.545626797571
$Li_6(H_2)_3$	2	Li_6 (ghost)	-45.127201810533

$Li_6(H_2)_3$	2	$3H_2$ (ghost)	-3.54560919062
$Li_6(H_2)_3$	3	$Li_6(H_2)_3$ (Complex)	-48.680971706338
$Li_6(H_2)_3$	3	Li_6 (in complex)	-45.126528815438
$Li_6(H_2)_3$	3	$3H_2$ (in complex)	-3.545484135352
$Li_6(H_2)_3$	3	Li_6 (ghost)	-45.127236254437
$Li_6(H_2)_3$	3	$3H_2$ (ghost)	-3.545470217295
$Li_6(H_2)_3$	4	$Li_6(H_2)_3$ (Complex)	-48.680720254334
$Li_6(H_2)_3$	4	Li_6 (in complex)	-45.12649348082
$Li_6(H_2)_3$	4	$3H_2$ (in complex)	-3.545405490754
$Li_6(H_2)_3$	4	Li_6 (ghost)	-45.12713244871
$Li_6(H_2)_3$	4	$3H_2$ (ghost)	-3.545396066965
$Li_6(H_2)_3$	5	$Li_6(H_2)_3$ (Complex)	-48.680183427657
$Li_6(H_2)_3$	5	Li_6 (in complex)	-45.126508594534
$Li_6(H_2)_3$	5	$3H_2$ (in complex)	-3.54535146685
$Li_6(H_2)_3$	5	Li_6 (ghost)	-45.127020593465
$Li_6(H_2)_3$	5	$3H_2$ (ghost)	-3.545347164202
$Li_6(H_2)_3$	6	$Li_6(H_2)_3$ (Complex)	-48.674102688588
$Li_6(H_2)_3$	6	Li_6 (in complex)	-45.126591340544
$Li_6(H_2)_3$	6	$3H_2$ (in complex)	-3.545428190756
$Li_6(H_2)_3$	6	Li_6 (ghost)	-45.126781302668
$Li_6(H_2)_3$	6	$3H_2$ (ghost)	-3.545438469562
$Li_6(H_2)_4$	0	$Li_6(H_2)_4$ (Complex)	-49.868617753937
$Li_6(H_2)_4$	0	Li_6 (in complex)	-45.126580395765
$Li_6(H_2)_4$	0	$4H_2$ (in complex)	-4.72723308896
$Li_6(H_2)_4$	0	Li_6 (ghost)	-45.127585950643
$Li_6(H_2)_4$	0	$4H_2$ (ghost)	-4.727217160735
$Li_6(H_2)_4$	1	$Li_6(H_2)_4$ (Complex)	-49.86843991907
$Li_6(H_2)_4$	1	Li_6 (in complex)	-45.126565842864

$Li_6(H_2)_4$	1	$4H_2$ (in complex)	-4.727255948358
$Li_6(H_2)_4$	1	Li_6 (ghost)	-45.127498190419
$Li_6(H_2)_4$	1	$4H_2$ (ghost)	-4.727227259364
$Li_6(H_2)_4$	2	$Li_6(H_2)_4$ (Complex)	-49.868218836578
$Li_6(H_2)_4$	2	Li_6 (in complex)	-45.126569713546
$Li_6(H_2)_4$	2	$4H_2$ (in complex)	-4.727180188267
$Li_6(H_2)_4$	2	Li_6 (ghost)	-45.127482839379
$Li_6(H_2)_4$	2	$4H_2$ (ghost)	-4.727165081046
$Li_6(H_2)_4$	3	$Li_6(H_2)_4$ (Complex)	-49.868295864037
$Li_6(H_2)_4$	3	Li_6 (in complex)	-45.126579173322
$Li_6(H_2)_4$	3	$4H_2$ (in complex)	-4.727375793831
$Li_6(H_2)_4$	3	Li_6 (ghost)	-45.127438498667
$Li_6(H_2)_4$	3	$4H_2$ (ghost)	-4.727356663339
$Li_6(H_2)_4$	4	$Li_6(H_2)_4$ (Complex)	-49.868308138542
$Li_6(H_2)_4$	4	Li_6 (in complex)	-45.126582304524
$Li_6(H_2)_4$	4	$4H_2$ (in complex)	-4.727374138415
$Li_6(H_2)_4$	4	Li_6 (ghost)	-45.127432158355
$Li_6(H_2)_4$	4	$4H_2$ (ghost)	-4.727353091285
$Li_6(H_2)_4$	5	$Li_6(H_2)_4$ (Complex)	-49.868059041927
$Li_6(H_2)_4$	5	Li_6 (in complex)	-45.126568308167
$Li_6(H_2)_4$	5	$4H_2$ (in complex)	-4.727250830129
$Li_6(H_2)_4$	5	Li_6 (ghost)	-45.127407368831
$Li_6(H_2)_4$	5	$4H_2$ (ghost)	-4.727233584908
$Li_6(H_2)_4$	6	$Li_6(H_2)_4$ (Complex)	-49.862804108198
$Li_6(H_2)_4$	6	Li_6 (in complex)	-45.126504678476
$Li_6(H_2)_4$	6	$4H_2$ (in complex)	-4.727254625086
$Li_6(H_2)_4$	6	Li_6 (ghost)	-45.127183365353
$Li_6(H_2)_4$	6	$4H_2$ (ghost)	-4.727248760468

$Li_6(H_2)_4$	7	$Li_6(H_2)_4$ (Complex)	-49.862296001885
$Li_6(H_2)_4$	7	Li_6 (in complex)	-45.126514386969
$Li_6(H_2)_4$	7	$4H_2$ (in complex)	-4.727167110923
$Li_6(H_2)_4$	7	Li_6 (ghost)	-45.127080832282
$Li_6(H_2)_4$	7	$4H_2$ (ghost)	-4.727167860397
$Li_6(H_2)_4$	8	$Li_6(H_2)_4$ (Complex)	-49.856176751589
$Li_6(H_2)_4$	8	Li_6 (in complex)	-45.12662407368
$Li_6(H_2)_4$	8	$4H_2$ (in complex)	-4.727241991081
$Li_6(H_2)_4$	8	Li_6 (ghost)	-45.126842553358
$Li_6(H_2)_4$	8	$4H_2$ (ghost)	-4.727258203885

Table S3. Total electronic energies and counterpoise components at the wB97X-2-D3BJ/def2-TZVPPD level of theory. All values are reported in atomic units (a.u.).

System	Isomer	Calculation Component	Electronic Energy
		H_2 (optimized isolated)	-1.153887646348
		Li_6 (optimized isolated)	-44.909076553326
$Li_6(H_2)_1$	0	$Li_6(H_2)_1$ (Complex)	-46.07074980812
$Li_6(H_2)_1$	0	Li_6 (in complex)	-44.908877333569
$Li_6(H_2)_1$	0	H_2 (in complex)	-1.153759663057
$Li_6(H_2)_1$	0	Li_6 (ghost)	-44.909757515959
$Li_6(H_2)_1$	0	H_2 (ghost)	-1.153810575399
$Li_6(H_2)_1$	1	$Li_6(H_2)_1$ (Complex)	-46.063495712598
$Li_6(H_2)_1$	1	Li_6 (in complex)	-44.908971481818
$Li_6(H_2)_1$	1	H_2 (in complex)	-1.153870056757
$Li_6(H_2)_1$	1	Li_6 (ghost)	-44.909243742784
$Li_6(H_2)_1$	1	H_2 (ghost)	-1.153902160646
$Li_6(H_2)_2$	0	$Li_6(H_2)_2$ (Complex)	-47.231552452012
$Li_6(H_2)_2$	0	Li_6 (in complex)	-44.908932987842
$Li_6(H_2)_2$	0	$2H_2$ (in complex)	-2.307566785347
$Li_6(H_2)_2$	0	Li_6 (ghost)	-44.910505755016
$Li_6(H_2)_2$	0	$2H_2$ (ghost)	-2.307674170432
$Li_6(H_2)_2$	1	$Li_6(H_2)_2$ (Complex)	-47.225752771349
$Li_6(H_2)_2$	1	Li_6 (in complex)	-44.908882221628
$Li_6(H_2)_2$	1	$2H_2$ (in complex)	-2.307849795906
$Li_6(H_2)_2$	1	Li_6 (ghost)	-44.910095266632
$Li_6(H_2)_2$	1	$2H_2$ (ghost)	-2.307911783175
$Li_6(H_2)_2$	2	$Li_6(H_2)_2$ (Complex)	-47.225185342561
$Li_6(H_2)_2$	2	Li_6 (in complex)	-44.908814146902
$Li_6(H_2)_2$	2	$2H_2$ (in complex)	-2.307640760517
$Li_6(H_2)_2$	2	Li_6 (ghost)	-44.909913078171

$Li_6(H_2)_2$	2	$2H_2$ (ghost)	-2.307723211968
$Li_6(H_2)_2$	3	$Li_6(H_2)_2$ (Complex)	-47.225554136276
$Li_6(H_2)_2$	3	Li_6 (in complex)	-44.908921073918
$Li_6(H_2)_2$	3	$2H_2$ (in complex)	-2.307940386147
$Li_6(H_2)_2$	3	Li_6 (ghost)	-44.909975123738
$Li_6(H_2)_2$	3	$2H_2$ (ghost)	-2.307998808561
$Li_6(H_2)_2$	4	$Li_6(H_2)_2$ (Complex)	-47.218260698542
$Li_6(H_2)_2$	4	Li_6 (in complex)	-44.908754113326
$Li_6(H_2)_2$	4	$2H_2$ (in complex)	-2.307797451458
$Li_6(H_2)_2$	4	Li_6 (ghost)	-44.909403044314
$Li_6(H_2)_2$	4	$2H_2$ (ghost)	-2.307868006249
$Li_6(H_2)_2$	5	$Li_6(H_2)_2$ (Complex)	-47.217791463245
$Li_6(H_2)_2$	5	Li_6 (in complex)	-44.908993025638
$Li_6(H_2)_2$	5	$2H_2$ (in complex)	-2.307757327217
$Li_6(H_2)_2$	5	Li_6 (ghost)	-44.909349227418
$Li_6(H_2)_2$	5	$2H_2$ (ghost)	-2.307809080192
$Li_6(H_2)_3$	0	$Li_6(H_2)_3$ (Complex)	-48.386544351055
$Li_6(H_2)_3$	0	Li_6 (in complex)	-44.908937710528
$Li_6(H_2)_3$	0	$3H_2$ (in complex)	-3.461665864417
$Li_6(H_2)_3$	0	Li_6 (ghost)	-44.910818403476
$Li_6(H_2)_3$	0	$3H_2$ (ghost)	-3.461786028271
$Li_6(H_2)_3$	1	$Li_6(H_2)_3$ (Complex)	-48.385965203571
$Li_6(H_2)_3$	1	Li_6 (in complex)	-44.908891459101
$Li_6(H_2)_3$	1	$3H_2$ (in complex)	-3.461452968092
$Li_6(H_2)_3$	1	Li_6 (ghost)	-44.910650652543
$Li_6(H_2)_3$	1	$3H_2$ (ghost)	-3.461590680415
$Li_6(H_2)_3$	2	$Li_6(H_2)_3$ (Complex)	-48.380717845453
$Li_6(H_2)_3$	2	Li_6 (in complex)	-44.908916994135

$Li_6(H_2)_3$	2	$3H_2$ (in complex)	-3.462240489251
$Li_6(H_2)_3$	2	Li_6 (ghost)	-44.91030508976
$Li_6(H_2)_3$	2	$3H_2$ (ghost)	-3.462305282233
$Li_6(H_2)_3$	3	$Li_6(H_2)_3$ (Complex)	-48.380703504856
$Li_6(H_2)_3$	3	Li_6 (in complex)	-44.908883072004
$Li_6(H_2)_3$	3	$3H_2$ (in complex)	-3.461978239486
$Li_6(H_2)_3$	3	Li_6 (ghost)	-44.910367111395
$Li_6(H_2)_3$	3	$3H_2$ (ghost)	-3.462051597234
$Li_6(H_2)_3$	4	$Li_6(H_2)_3$ (Complex)	-48.380195764094
$Li_6(H_2)_3$	4	Li_6 (in complex)	-44.908814024413
$Li_6(H_2)_3$	4	$3H_2$ (in complex)	-3.461744575989
$Li_6(H_2)_3$	4	Li_6 (ghost)	-44.91022335907
$Li_6(H_2)_3$	4	$3H_2$ (ghost)	-3.461837836143
$Li_6(H_2)_3$	5	$Li_6(H_2)_3$ (Complex)	-48.37951720612
$Li_6(H_2)_3$	5	Li_6 (in complex)	-44.908819497657
$Li_6(H_2)_3$	5	$3H_2$ (in complex)	-3.461530723124
$Li_6(H_2)_3$	5	Li_6 (ghost)	-44.91000015044
$Li_6(H_2)_3$	5	$3H_2$ (ghost)	-3.461632149453
$Li_6(H_2)_3$	6	$Li_6(H_2)_3$ (Complex)	-48.372157661439
$Li_6(H_2)_3$	6	Li_6 (in complex)	-44.908963328413
$Li_6(H_2)_3$	6	$3H_2$ (in complex)	-3.461641069601
$Li_6(H_2)_3$	6	Li_6 (ghost)	-44.909475566699
$Li_6(H_2)_3$	6	$3H_2$ (ghost)	-3.461714652138
$Li_6(H_2)_4$	0	$Li_6(H_2)_4$ (Complex)	-49.54153222038
$Li_6(H_2)_4$	0	Li_6 (in complex)	-44.908935878082
$Li_6(H_2)_4$	0	$4H_2$ (in complex)	-4.615776544295
$Li_6(H_2)_4$	0	Li_6 (ghost)	-44.911119624715
$Li_6(H_2)_4$	0	$4H_2$ (ghost)	-4.615908656524

$Li_6(H_2)_4$	1	$Li_6(H_2)_4$ (Complex)	-49.541345362024
$Li_6(H_2)_4$	1	Li_6 (in complex)	-44.908938388859
$Li_6(H_2)_4$	1	$4H_2$ (in complex)	-4.615806057155
$Li_6(H_2)_4$	1	Li_6 (ghost)	-44.911010685522
$Li_6(H_2)_4$	1	$4H_2$ (ghost)	-4.615925399678
$Li_6(H_2)_4$	2	$Li_6(H_2)_4$ (Complex)	-49.540964179849
$Li_6(H_2)_4$	2	Li_6 (in complex)	-44.908895559726
$Li_6(H_2)_4$	2	$4H_2$ (in complex)	-4.615560246523
$Li_6(H_2)_4$	2	Li_6 (ghost)	-44.910945821172
$Li_6(H_2)_4$	2	$4H_2$ (ghost)	-4.615709295269
$Li_6(H_2)_4$	3	$Li_6(H_2)_4$ (Complex)	-49.541211958903
$Li_6(H_2)_4$	3	Li_6 (in complex)	-44.908955087181
$Li_6(H_2)_4$	3	$4H_2$ (in complex)	-4.615952119709
$Li_6(H_2)_4$	3	Li_6 (ghost)	-44.910878934981
$Li_6(H_2)_4$	3	$4H_2$ (ghost)	-4.616077683745
$Li_6(H_2)_4$	4	$Li_6(H_2)_4$ (Complex)	-49.54119202882
$Li_6(H_2)_4$	4	Li_6 (in complex)	-44.908960908272
$Li_6(H_2)_4$	4	$4H_2$ (in complex)	-4.615946687434
$Li_6(H_2)_4$	4	Li_6 (ghost)	-44.91087221737
$Li_6(H_2)_4$	4	$4H_2$ (ghost)	-4.616070611257
$Li_6(H_2)_4$	5	$Li_6(H_2)_4$ (Complex)	-49.540784683692
$Li_6(H_2)_4$	5	Li_6 (in complex)	-44.908905942568
$Li_6(H_2)_4$	5	$4H_2$ (in complex)	-4.615643292255
$Li_6(H_2)_4$	5	Li_6 (ghost)	-44.910821718081
$Li_6(H_2)_4$	5	$4H_2$ (ghost)	-4.615788485403
$Li_6(H_2)_4$	6	$Li_6(H_2)_4$ (Complex)	-49.534541898602
$Li_6(H_2)_4$	6	Li_6 (in complex)	-44.908808192719
$Li_6(H_2)_4$	6	$4H_2$ (in complex)	-4.615654346294
$Li_6(H_2)_4$	6	Li_6 (ghost)	-44.910308283167

$Li_6(H_2)_4$	6	$4H_2$ (ghost)	-4.61576524333
$Li_6(H_2)_4$	7	$Li_6(H_2)_4$ (Complex)	-49.533873520995
$Li_6(H_2)_4$	7	Li_6 (in complex)	-44.908809131194
$Li_6(H_2)_4$	7	$4H_2$ (in complex)	-4.615417690227
$Li_6(H_2)_4$	7	Li_6 (ghost)	-44.910118624657
$Li_6(H_2)_4$	7	$4H_2$ (ghost)	-4.615539639172
$Li_6(H_2)_4$	8	$Li_6(H_2)_4$ (Complex)	-49.526507985284
$Li_6(H_2)_4$	8	Li_6 (in complex)	-44.908994644747
$Li_6(H_2)_4$	8	$4H_2$ (in complex)	-4.615529811332
$Li_6(H_2)_4$	8	Li_6 (ghost)	-44.909560138603
$Li_6(H_2)_4$	8	$4H_2$ (ghost)	-4.615615904516

Table S4. Zero-point energies (ZPE), thermal enthalpy corrections (H_{corr}), and entropy terms (TS) at the wB97X-D4rev/def2-TZVPPD level. All values reported in atomic units (a.u.) at 298.15 K and 1 atm.

System	Isomer	Calculation Component	ZPE	H_{corr}	TS
		H_2 (optimized isolated)	0.01011475	0.00236045	0.01479268
		Li_6 (optimized isolated)	0.0064041	0.00911151	0.04064725
$Li_6(H_2)_1$	0	$Li_6(H_2)_1$ (Complex)	0.0197881	0.01147471	0.04605105
$Li_6(H_2)_1$	0	Li_6 (in complex)	0.00645121	0.00908261	0.04057488
$Li_6(H_2)_1$	0	H_2 (in complex)	0.00973969	0.00236045	0.01482258
$Li_6(H_2)_1$	1	$Li_6(H_2)_1$ (Complex)	0.01803403	0.01249656	0.04837152
$Li_6(H_2)_1$	1	Li_6 (in complex)	0.00639418	0.00912059	0.04066306
$Li_6(H_2)_1$	1	H_2 (in complex)	0.01000801	0.00236045	0.01480114
$Li_6(H_2)_2$	0	$Li_6(H_2)_2$ (Complex)	0.03311436	0.01386007	0.05077169
$Li_6(H_2)_2$	0	Li_6 (in complex)	0.00648746	0.0090557	0.04050484
$Li_6(H_2)_2$	0	$2H_2$ (in complex)	0.02308197	0.00347216	0.02400287
$Li_6(H_2)_2$	1	$Li_6(H_2)_2$ (Complex)	0.03126786	0.01494769	0.05331639
$Li_6(H_2)_2$	1	Li_6 (in complex)	0.00644875	0.0090843	0.04123348
$Li_6(H_2)_2$	1	$2H_2$ (in complex)	0.02279882	0.00450103	0.02450167
$Li_6(H_2)_2$	2	$Li_6(H_2)_2$ (Complex)	0.03132576	0.01495256	0.05333435
$Li_6(H_2)_2$	2	Li_6 (in complex)	0.00644471	0.0090889	0.04124187
$Li_6(H_2)_2$	2	$2H_2$ (in complex)	0.02267341	0.00373908	0.02422811
$Li_6(H_2)_2$	3	$Li_6(H_2)_2$ (Complex)	0.03102078	0.01514719	0.05395885
$Li_6(H_2)_2$	3	Li_6 (in complex)	0.00644534	0.00908553	0.04123642
$Li_6(H_2)_2$	3	$2H_2$ (in complex)	0.02297803	0.00445021	0.02423398
$Li_6(H_2)_2$	4	$Li_6(H_2)_2$ (Complex)	0.03050757	0.01526482	0.05380374
$Li_6(H_2)_2$	4	Li_6 (in complex)	0.00635578	0.00914874	0.0413733
$Li_6(H_2)_2$	4	$2H_2$ (in complex)	0.02284614	0.00444846	0.02404214

$Li_6(H_2)_2$	5	$Li_6(H_2)_2$ (Complex)	0.02870989	0.01662747	0.05758389
$Li_6(H_2)_2$	5	Li_6 (in complex)	0.00640575	0.0091134	0.04130938
$Li_6(H_2)_2$	5	$2H_2$ (in complex)	0.02167517	0.00437592	0.02673182
$Li_6(H_2)_3$	0	$Li_6(H_2)_3$ (Complex)	0.04451885	0.01740088	0.05820714
$Li_6(H_2)_3$	0	Li_6 (in complex)	0.00648505	0.00905719	0.04116266
$Li_6(H_2)_3$	0	$3H_2$ (in complex)	0.03555387	0.00545147	0.02985368
$Li_6(H_2)_3$	1	$Li_6(H_2)_3$ (Complex)	0.0445227	0.01744138	0.05829787
$Li_6(H_2)_3$	1	Li_6 (in complex)	0.00648471	0.00905925	0.04116645
$Li_6(H_2)_3$	1	$3H_2$ (in complex)	0.03539115	0.00468096	0.02882629
$Li_6(H_2)_3$	2	$Li_6(H_2)_3$ (Complex)	0.04243653	0.0186554	0.06123704
$Li_6(H_2)_3$	2	Li_6 (in complex)	0.00644456	0.00908623	0.0412381
$Li_6(H_2)_3$	2	$3H_2$ (in complex)	0.0349804	0.00754435	0.03274671
$Li_6(H_2)_3$	3	$Li_6(H_2)_3$ (Complex)	0.0425958	0.01854962	0.06092598
$Li_6(H_2)_3$	3	Li_6 (in complex)	0.00644827	0.00908473	0.04123425
$Li_6(H_2)_3$	3	$3H_2$ (in complex)	0.03469835	0.00683195	0.03133736
$Li_6(H_2)_3$	4	$Li_6(H_2)_3$ (Complex)	0.04276303	0.01846826	0.06066811
$Li_6(H_2)_3$	4	Li_6 (in complex)	0.00644557	0.00908839	0.04124117
$Li_6(H_2)_3$	4	$3H_2$ (in complex)	0.03473819	0.00592641	0.03051136
$Li_6(H_2)_3$	5	$Li_6(H_2)_3$ (Complex)	0.0420567	0.0190559	0.06244267
$Li_6(H_2)_3$	5	Li_6 (in complex)	0.00645269	0.00908423	0.04123604
$Li_6(H_2)_3$	5	$3H_2$ (in complex)	0.03428264	0.00631646	0.03369986
$Li_6(H_2)_3$	6	$Li_6(H_2)_3$ (Complex)	0.03973804	0.02050972	0.06610666
$Li_6(H_2)_3$	6	Li_6 (in complex)	0.00640183	0.00911694	0.04131335
$Li_6(H_2)_3$	6	$3H_2$ (in complex)	0.03305857	0.00610259	0.03268299
$Li_6(H_2)_4$	0	$Li_6(H_2)_4$ (Complex)	0.05590271	0.02096508	0.06570552

$Li_6(H_2)_4$	0	Li_6 (in complex)	0.00648495	0.00905728	0.04116272
$Li_6(H_2)_4$	0	$4H_2$ (in complex)	0.0468561	0.00724381	0.03448718
$Li_6(H_2)_4$	1	$Li_6(H_2)_4$ (Complex)	0.05545376	0.02131545	0.06692682
$Li_6(H_2)_4$	1	Li_6 (in complex)	0.00647787	0.00906165	0.04117249
$Li_6(H_2)_4$	1	$4H_2$ (in complex)	0.04680025	0.00727145	0.03450796
$Li_6(H_2)_4$	2	$Li_6(H_2)_4$ (Complex)	0.05588892	0.02101811	0.06580999
$Li_6(H_2)_4$	2	Li_6 (in complex)	0.00648512	0.00905885	0.04116594
$Li_6(H_2)_4$	2	$4H_2$ (in complex)	0.04667962	0.00647518	0.03326173
$Li_6(H_2)_4$	3	$Li_6(H_2)_4$ (Complex)	0.05569288	0.02115107	0.06634762
$Li_6(H_2)_4$	3	Li_6 (in complex)	0.00647865	0.00906061	0.04117053
$Li_6(H_2)_4$	3	$4H_2$ (in complex)	0.04661277	0.00741925	0.03509245
$Li_6(H_2)_4$	4	$Li_6(H_2)_4$ (Complex)	0.05559955	0.02120907	0.0665369
$Li_6(H_2)_4$	4	Li_6 (in complex)	0.00647852	0.0090605	0.04117041
$Li_6(H_2)_4$	4	$4H_2$ (in complex)	0.04662366	0.00739936	0.03496044
$Li_6(H_2)_4$	5	$Li_6(H_2)_4$ (Complex)	0.05569196	0.02117529	0.06634815
$Li_6(H_2)_4$	5	Li_6 (in complex)	0.0064812	0.00906101	0.04117058
$Li_6(H_2)_4$	5	$4H_2$ (in complex)	0.04654054	0.00657051	0.03355043
$Li_6(H_2)_4$	6	$Li_6(H_2)_4$ (Complex)	0.05348818	0.02258699	0.06993071
$Li_6(H_2)_4$	6	Li_6 (in complex)	0.00645458	0.0090833	0.0412337
$Li_6(H_2)_4$	6	$4H_2$ (in complex)	0.04554923	0.00812654	0.0379691
$Li_6(H_2)_4$	7	$Li_6(H_2)_4$ (Complex)	0.0529813	0.02302234	0.07128727
$Li_6(H_2)_4$	7	Li_6 (in complex)	0.00645214	0.00908521	0.04123661
$Li_6(H_2)_4$	7	$4H_2$ (in complex)	0.04508473	0.00851553	0.0406447
$Li_6(H_2)_4$	8	$Li_6(H_2)_4$ (Complex)	0.05027413	0.02478277	0.07595696
$Li_6(H_2)_4$	8	Li_6 (in complex)	0.00641114	0.00911061	0.04130323
$Li_6(H_2)_4$	8	$4H_2$ (in complex)	0.04360913	0.00755279	0.03678902

Table S5. Energetic components and relative stabilities (kcal/mol) for $Li_6(H_2)_n$ complexes at the wB97X-D4rev/def2-TZVPPD level of theory. Values are derived from electronic energies and ZPE corrections. $\Delta E_{ads,Total}$ represents the final corrected adsorption energy.

System	Isomer	E_{int}	E_{def}	δ_{CP}	ΔZPE	$\Delta E_{ads,Total}$	ΔΔE
$Li_6(H_2)_1$	0 (GM)	-5.091	0.205	0.584	2.051	-2.25	0
$Li_6(H_2)_1$	1	-0.411	0.077	0.191	0.951	0.808	3.058
$Li_6(H_2)_2$	0 (GM)	-9.446	0.221	1.054	4.067	-4.104	0
$Li_6(H_2)_2$	3	-5.455	-0.006	0.698	2.753	-2.01	2.094
$Li_6(H_2)_2$	1	-5.661	0.075	0.8	2.908	-1.877	2.226
$Li_6(H_2)_2$	2	-5.478	0.249	0.741	2.944	-1.544	2.56
$Li_6(H_2)_2$	5	-0.653	0.064	0.256	1.303	0.969	5.073
$Li_6(H_2)_2$	4	-1.072	0.188	0.451	2.431	1.998	6.102
$Li_6(H_2)_3$	0 (GM)	-10.003	0.085	1.256	4.876	-3.786	0
$Li_6(H_2)_3$	1	-9.802	0.248	1.19	4.878	-3.485	0.301
$Li_6(H_2)_3$	2	-5.999	-0.262	0.912	3.569	-1.78	2.006
$Li_6(H_2)_3$	3	-6.176	-0.076	0.977	3.669	-1.606	2.18
$Li_6(H_2)_3$	5	-5.752	0.244	0.805	3.331	-1.373	2.414
$Li_6(H_2)_3$	4	-6.047	0.114	0.943	3.774	-1.217	2.569
$Li_6(H_2)_3$	6	-0.975	0.085	0.368	1.876	1.354	5.14
$Li_6(H_2)_4$	1 (GM)	-10.417	-0.074	1.375	5.391	-3.725	0
$Li_6(H_2)_4$	4	-10.219	-0.176	1.277	5.482	-3.635	0.09
$Li_6(H_2)_4$	3	-10.231	-0.176	1.286	5.541	-3.58	0.145
$Li_6(H_2)_4$	0	-10.555	-0.054	1.453	5.672	-3.482	0.242
$Li_6(H_2)_4$	5	-10.188	0.049	1.293	5.54	-3.306	0.419
$Li_6(H_2)_4$	2	-10.359	0.108	1.38	5.664	-3.208	0.517
$Li_6(H_2)_4$	7	-6.053	0.251	0.898	3.839	-1.065	2.66
$Li_6(H_2)_4$	6	-6.325	0.103	1.011	4.157	-1.053	2.671
$Li_6(H_2)_4$	8	-1.245	0.064	0.409	2.14	1.369	5.094

Table S6. Thermodynamic adsorption properties and Boltzmann population distribution for $Li_6(H_2)_n$ complexes. All energy values are reported in kcal/mol at 298.15 K and 1 atm. ΔΔG represents the relative stability compared to the Global Minimum (GM) of each group.

System	Isomer	ΔU	ΔH	TΔS	ΔG	% Dist	ΔΔG
$Li_6(H_2)_1$	0 (GM)	-2.25	-2.84	-5.89	3.05	97.78	0
	1	1.45	0.86	-4.44	5.29	2.22	2.24
$Li_6(H_2)_2$	0 (GM)	-4.09	-5.27	-12.21	6.94	71.2	0
	3	-1.18	-2.37	-10.21	7.84	15.54	0.9
	1	-1.18	-2.36	-10.62	8.25	7.77	1.31
	2	-0.84	-2.03	-10.6	8.58	4.49	1.64
	5	2.72	1.54	-7.94	9.48	0.99	2.53
	4	2.9	1.71	-10.31	12.02	0.01	5.08
$Li_6(H_2)_3$	0 (GM)	-3.03	-4.81	-16.83	12.02	42.8	0
	1	-2.7	-4.48	-16.77	12.29	27.18	0.27
	5	0.42	-1.35	-14.17	12.82	11.2	0.79
	2	-0.24	-2.01	-14.93	12.91	9.5	0.89
	3	-0.13	-1.9	-15.12	13.22	5.7	1.19
	4	0.21	-1.57	-15.28	13.72	2.45	1.69
	6	4.06	2.29	-11.87	14.16	1.17	2.13
$Li_6(H_2)_4$	1 (GM)	-1.99	-4.36	-20.64	16.28	31.12	0
	4	-1.97	-4.34	-20.88	16.55	19.82	0.27
	3	-1.95	-4.32	-21	16.68	15.72	0.4
	5	-1.66	-4.03	-21	16.97	9.64	0.69
	0	-1.97	-4.34	-21.41	17.07	8.22	0.79
	7	1.74	-0.63	-17.9	17.27	5.8	0.99
	2	-1.66	-4.03	-21.34	17.31	5.46	1.03
	6	1.48	-0.89	-18.75	17.86	2.15	1.58
	8	5.28	2.91	-14.97	17.88	2.08	1.6

Table S7. Geometric descriptors for isolated species and $Li_6(H_2)_n$ complexes at the wB97X-D4rev/def2-TZVPPD level of theory. Distances are reported in Angstroms (Å). Isomers are ordered according to their thermodynamic stability (ΔΔG) at 298.15 K. RMSD is calculated for the Li_6 core relative to the isolated cluster.

System	Isomer	$r_{H–H}$	$d_{Li–H}$	$d_{H_2–H_2}$	$r_{Li–Li}$	RMSD
$Li_6(H_2)_1$	0 (GM)	0.755	1.987	—	3.298	0.0315
	1	0.746	2.53	—	3.313	0.0518
$Li_6(H_2)_2$	0 (GM)	0.753	2.011	6.489	3.288	0.0178
	3	0.749	2.978	3.083	3.299	0.0282
	1	0.749	2.861	2.998	3.298	0.0315
	2	0.75	2.286	6.01	3.3	0.0497
	5	0.745	2.842	10.738	3.31	0.0125
	4	0.747	2.417	2.829	3.323	0.103
$Li_6(H_2)_3$	0 (GM)	0.75	2.591	3.02	3.289	0.0179
	1	0.751	2.235	6.108	3.29	0.032
	5	0.748	2.586	6.277	3.299	0.0319
	2	0.747	3.221	3.024	3.299	0.0285
	3	0.748	3.17	3.038	3.298	0.0315
	4	0.748	2.789	3.026	3.3	0.0492
	6	0.745	2.924	7.761	3.312	0.0407
$Li_6(H_2)_4$	1 (GM)	0.749	2.91	3.048	3.29	0.0232
	4	0.748	3.004	3.119	3.29	0.0179
	3	0.748	3.007	3.12	3.29	0.0187
	5	0.749	2.689	3.135	3.291	0.0314
	0	0.749	2.887	3.035	3.289	0.018
	7	0.747	2.742	6.213	3.3	0.0413
	2	0.749	2.627	3.041	3.29	0.0301
	6	0.747	2.904	3.061	3.299	0.0328
	8	0.744	3.117	7.964	3.31	0.0062

Table S8. Magnetic aromaticity indices (NICS) for $Li_6(H_2)_n$ complexes at the wB97X-D4rev/def2-TZVPPD level of theory. Isotropic shielding (σ_{iso}) and NICS(0) values are reported in ppm. Isomers are ordered according to their thermodynamic stability (ΔΔG) at 298.15 K.

System	Isomer	σ_{iso} (ppm)	NICS(0) (ppm)	Aromaticity Status
$Li_6(H_2)_1$	0 (GM)	10.74	-10.74	Strongly Aromatic
	1	1.73	-1.73	Quenched
$Li_6(H_2)_2$	0 (GM)	13.98	-13.98	Strongly Aromatic
	3	10.49	-10.49	Strongly Aromatic
	1	10.59	-10.59	Strongly Aromatic
	2	9.95	-9.95	Aromatic
	5	1.67	-1.67	Quenched
	4	0.51	-0.51	Quenched
$Li_6(H_2)_3$	0 (GM)	13.85	-13.85	Strongly Aromatic
	1	13.39	-13.39	Strongly Aromatic
	5	9.95	-9.95	Aromatic
	2	10.35	-10.35	Strongly Aromatic
	3	10.45	-10.45	Strongly Aromatic
	4	9.85	-9.85	Aromatic
	6	1.08	-1.08	Quenched
$Li_6(H_2)_4$	1 (GM)	13.7	-13.7	Strongly Aromatic
	4	13.71	-13.71	Strongly Aromatic
	3	13.71	-13.71	Strongly Aromatic
	5	13.3	-13.3	Strongly Aromatic
	0	13.74	-13.74	Strongly Aromatic
	7	9.61	-9.61	Aromatic
	2	13.31	-13.31	Strongly Aromatic
	6	9.88	-9.88	Aromatic
	8	1.25	-1.25	Quenched

Table S9. Harmonic stretching frequencies (ν) and classification of adsorbed H_2 molecules. All frequencies are reported in cm^{-1}. Isomers are ordered according to their thermodynamic stability (ΔΔG) at 298.15 K. Reference isolated H_2 (gas) frequency: 4401 cm^{-1}.

System	Isomer	Activated ν	Spectator ν	Classification
$Li_6(H_2)_1$	0 (GM)	4219	—	1 Activated
	1	—	4368	1 Spectator
$Li_6(H_2)_2$	0 (GM)	4244, 4246	—	2 Activated
	3	4238	4404	1 Act / 1 Spec
	1	4226	4397	1 Act / 1 Spec
	2	4222	4380	1 Act / 1 Spec
	5	—	4394, 4395	2 Spectators
	4	—	4352, 4352	2 Spectators
$Li_6(H_2)_3$	0 (GM)	4247, 4250	4404	2 Act / 1 Spec
	1	4246, 4248	4392	2 Act / 1 Spec
	5	4224	4400, 4401	1 Act / 2 Spec
	2	4241	4400, 4405	1 Act / 2 Spec
	3	4229	4402, 4403	1 Act / 2 Spec
	4	4225	4386, 4402	1 Act / 2 Spec
	6	—	4393, 4406, 4407	3 Spectators
$Li_6(H_2)_4$	1 (GM)	4252, 4257	4406, 4407	2 Act / 2 Spec
	4	4259, 4261	4411, 4411	2 Act / 2 Spec
	3	4249, 4270	4411, 4412	2 Act / 2 Spec
	5	4248, 4259	4396, 4411	2 Act / 2 Spec
	0	4249, 4252	4407, 4407	2 Act / 2 Spec
	7	4226	4402, 4410, 4412	1 Act / 3 Spec
	2	4247, 4250	4396, 4406	2 Act / 2 Spec
	6	4225	4404, 4405, 4405	1 Act / 3 Spec
	8	—	4412, 4412, 4412, 4412	4 Spectators

Table S10. Energy Decomposition Analysis (EDA) components for $Li_6(H_2)_n$ complexes, according to the Ziegler–Rauk scheme. All values are reported in kcal/mol. Isomers are ordered according to their thermodynamic stability (ΔΔG) at 298.15 K.

System	Isomer	E_{int}	E_{prep}	E_{bind}	E_{elstat}	E_{Pauli}	E_{orb}	E_{XC}	E_{disp}
$Li_6(H_2)_1$	0 (GM)	-4.35	0.12	-4.23	-9.34	13.96	-4.03	-3.91	-1.03
	1	-0.69	0.01	-0.68	-6.66	10.37	-1.64	-2.02	-0.74
$Li_6(H_2)_2$	0 (GM)	-7.95	0.31	-7.64	-17.06	25.25	-7.24	-7.19	-1.72
	3	-4.73	0.25	-4.48	-10.33	15.33	-4.09	-4.3	-1.34
	1	-4.86	0.26	-4.6	-11.17	16.72	-4.36	-4.63	-1.42
	2	-4.74	0.15	-4.59	-15.5	23.55	-5.52	-5.79	-1.48
	5	-0.96	0.05	-0.91	-8.1	12.47	-1.67	-2.61	-1.05
	4	-1.66	0.14	-1.52	-17.01	26.89	-4.74	-5.18	-1.62
$Li_6(H_2)_3$	0 (GM)	-8.34	0.44	-7.9	-18.81	27.87	-7.54	-7.88	-1.98
	1	-8.18	0.34	-7.84	-22.36	33.48	-8.44	-8.84	-2.01
	5	-4.91	0.18	-4.73	-16.94	25.64	-5.58	-6.38	-1.66
	2	-5.26	0.45	-4.81	-12.28	18.32	-4.46	-5.09	-1.75
	3	-5.19	0.4	-4.79	-12.84	19.22	-4.64	-5.3	-1.64
	4	-5.15	0.28	-4.87	-16.98	25.74	-5.75	-6.41	-1.75
	6	-1.19	0.09	-1.1	-10.78	16.55	-2.16	-3.53	-1.27
$Li_6(H_2)_4$	1 (GM)	-8.62	0.51	-8.11	-20.01	29.62	-7.68	-8.38	-2.16
	4	-8.49	0.44	-8.05	-18.97	27.88	-7.38	-7.96	-2.07
	3	-8.48	0.44	-8.04	-19.02	27.96	-7.39	-7.98	-2.05
	5	-8.43	0.32	-8.11	-22.93	34.17	-8.4	-9.12	-2.15
	0	-8.68	0.57	-8.11	-20.5	30.41	-7.84	-8.56	-2.18
	7	-5.06	0.22	-4.84	-18.89	28.58	-5.86	-7.1	-1.79
	2	-8.52	0.48	-8.04	-23.8	35.59	-8.66	-9.44	-2.21
	6	-5.26	0.34	-4.92	-18.22	27.54	-5.78	-6.95	-1.86
	8	-1.31	0.13	-1.18	-10.31	15.68	-1.82	-3.56	-1.31

The energy decomposition analysis (EDA) was performed according to the Ziegler–Rauk scheme to quantify the physical nature of the Li_6–nH_2 interaction:

E_{int} (Interaction Energy): Total electronic interaction energy between the fragments at the distorted geometry they adopt within the complex ($E_{int}=E_{elstat}+E_{Pauli}+E_{orb}+E_{XC}+E_{disp}$).

E_{prep} (Preparation Energy): The energetic penalty (positive value) required to deform the fragments from their isolated equilibrium geometries to the geometry they adopt in the complex.

E_{bind} (Binding Energy): The total stability of the complex relative to the isolated fragments, defined as $E_{bind}=E_{int}+E_{prep}$.

E_{elstat} (Electrostatic): Classical attractive Coulombic interaction between the unperturbed charge distributions of the fragments.

E_{Pauli} (Pauli Repulsion): The destabilizing energy contribution arising from the overlap of occupied orbitals, according to the Pauli exclusion principle.

E_{orb} (Orbital Interaction): Stabilization term due to charge transfer (occupied-virtual orbital mixing) and polarization effects.

E_{XC} (Exchange-Correlation): The change in the exchange-correlation energy resulting from the preparation of the fragments within the functional framework.

E_{disp} (Dispersion): Stabilization energy derived from long-range van der Waals forces, treated here via the D4 or D3BJ dispersion correction.

Table S11. Topological parameters of the electron density at the Bond Critical Points (BCP) for Li–H interactions in Global Minima. All values are reported in atomic units (a.u.) at the wB97X-D4rev/def2-TZVPPD level of theory. Only the most stable isomers according to Gibbs free energy (ΔG) are reported.

System	Isomer	Interaction	ρ(r)	$\nabla^2\rho(r)$	Characterization
$Li_6(H_2)_1$	0 (GM)	H_2 (1)	0.013	0.0821	Strong Physisorption
$Li_6(H_2)_2$	0 (GM)	H_2 (1)	0.0122	0.0767	Competitive Physisorption
		H_2 (2)	0.0122	0.0767	Competitive Physisorption
$Li_6(H_2)_3$	0 (GM)	H_2 (1)	0.0127	0.0765	Relaxed Physisorption
		H_2 (2)	0.0127	0.0765	Relaxed Physisorption
		H_2 (3)	0.0131	0.0827	Steric Confinement
$Li_6(H_2)_4$	1 (GM)	H_2 (1)	0.0125	0.0761	Relaxed Physisorption
		H_2 (2)	0.0125	0.0761	Relaxed Physisorption
		H_2 (3)	0.013	0.0818	Steric Confinement
		H_2 (4)	0.013	0.0818	Steric Confinement

QTAIM Definitions and Interpretation for Table S12.

ρ(r) (Electron Density): Quantifies the charge density at the Bond Critical Point (BCP). Values in the range of 0.012–0.013 a.u. are characteristic of weak closed-shell interactions, specifically physisorption in lithium-hydrogen systems.

$\nabla^2\rho(r)$ (Laplacian of Electron Density): A positive value ($\nabla 2\rho(r)>0$) indicates a depletion of electron density at the BCP, which is a hallmark of non-covalent interactions.

Steric Confinement: For n=3 and n=4, the emergence of "compressed" interactions (with slightly higher ρ and $\nabla 2\rho$) reflects the overcrowding of the first coordination sphere, a key factor in the saturation of the Li_6 cluster.

Table S12. Atomic Charges and Volumes from Bader Population Analysis (QTAIM) at the wB97X-D4/def2-TZVPPD level of theory. Only the most stable isomers according to Gibbs free energy (ΔG) are reported.

System	Atom / Type	Index	Charge (e)	Volume (Bohr³)
$Li_6(H_2)_1$	NNA	2	-1.071453	212.858
	NNA	3	-1.072079	212.929
	NNA	4	-1.071460	212.838
	NNA	8	-1.071885	212.884
	Li	1	0.798768	47.920
	Li	2	0.693126	89.111
	Li	3	0.789459	39.160
	Li	4	0.693090	89.107
	Li	5	0.693274	89.076
	Li	6	0.693326	89.084
	H	7	-0.037122	68.772
	H	8	-0.037045	68.772
$Li_6(H_2)_2$	NNA	1	-1.058989	210.435
	NNA	2	-1.058975	210.457
	NNA	6	-1.059426	210.524
	NNA	12	-1.059101	210.464
	Li	1	0.796181	39.230
	Li	2	0.694509	88.681
	Li	3	0.796088	39.248
	Li	4	0.694554	88.689
	Li	5	0.694591	88.704
	Li	6	0.694596	88.700
	H	7	-0.033443	68.390

System	Atom / Type	Index	Charge (e)	Volume (Bohr³)
	H	8	-0.033564	68.396
	H	9	-0.033428	68.380
	H	10	-0.033591	68.385
$Li_6(H_2)_3$	NNA	1	-1.063261	211.263
	NNA	2	-1.062953	211.244
	NNA	4	-1.051537	210.811
	NNA	15	-1.051764	210.836
	Li	1	0.797092	38.957
	Li	2	0.796009	39.333
	Li	3	0.696823	88.187
	Li	4	0.694856	88.484
	Li	5	0.696793	88.170
	Li	6	0.694900	88.470
	H (Act.)	7	-0.031001	68.959
	H (Act.)	8	-0.033813	68.947
	H (Act.)	9	-0.033577	68.384
	H (Act.)	10	-0.033136	68.348
	H (Spec.)	11	-0.009254	61.798
	H (Spec.)	12	-0.006177	69.513
$Li_6(H_2)_4$	NNA	2	-1.062305	212.827
	NNA	3	-1.045528	210.022
	NNA	9	-1.059832	212.994
	NNA	17	-1.052696	210.898

System	Atom / Type	Index	Charge (e)	Volume (Bohr³)
	Li	1	0.797236	39.193
	Li	2	0.697008	87.956
	Li	3	0.796841	39.080
	Li	4	0.695289	88.328
	Li	5	0.695734	88.289
	Li	6	0.694540	88.611
	H (Spec.)	7	-0.005978	69.398
	H (Spec.)	8	-0.009122	61.763
	H (Spec.)	9	-0.006084	68.848
	H (Spec.)	10	-0.008224	61.709
	H (Act.)	11	-0.032965	68.910
	H (Act.)	12	-0.031220	68.996
	H (Act.)	13	-0.033612	68.391
	H (Act.)	14	-0.029082	69.288

Table S13. Frontier molecular orbital indices (NO), energies, and HOMO-LUMO gaps for all $Li_6(H_2)_n$ isomers.

System/Isomer	idxH	HOMO (eV)	idxL	LUMO (eV)	Gap (eV)
$Li_6(H_2)_1$ iso_0	9	-4.9063	10	-0.0170	4.8893
$Li_6(H_2)_1$ iso_1	9	-4.8273	10	-0.2651	4.5622
$Li_6(H_2)_2$ iso_0	10	-4.9073	11	0.1307	5.0380
$Li_6(H_2)_2$ iso_1	10	-4.9121	11	-0.0089	4.9032
$Li_6(H_2)_2$ iso_2	10	-4.8358	11	0.0195	4.8553
$Li_6(H_2)_2$ iso_3	10	-4.9006	11	-0.0121	4.8885
$Li_6(H_2)_2$ iso_4	10	-4.7618	11	-0.2024	4.5594
$Li_6(H_2)_2$ iso_5	10	-4.7922	11	-0.2378	4.5544
$Li_6(H_2)_3$ iso_0	11	-4.9054	12	0.1390	5.0444
$Li_6(H_2)_3$ iso_1	11	-4.8423	12	0.2100	5.0523
$Li_6(H_2)_3$ iso_2	11	-4.9057	12	-0.0116	4.8941
$Li_6(H_2)_3$ iso_3	11	-4.9136	12	-0.0034	4.9102
$Li_6(H_2)_3$ iso_4	11	-4.8431	12	0.0256	4.8687
$Li_6(H_2)_3$ iso_5	11	-4.7966	12	0.0429	4.8395
$Li_6(H_2)_3$ iso_6	11	-4.7539	12	-0.2153	4.5386
$Li_6(H_2)_4$ iso_0	12	-4.9124	13	0.1494	5.0618
$Li_6(H_2)_4$ iso_1	12	-4.9032	13	0.1472	5.0504
$Li_6(H_2)_4$ iso_2	12	-4.8446	13	0.2161	5.0607
$Li_6(H_2)_4$ iso_3	12	-4.8987	13	0.1460	5.0447
$Li_6(H_2)_4$ iso_4	12	-4.9034	13	0.1470	5.0504
$Li_6(H_2)_4$ iso_5	12	-4.8423	13	0.2142	5.0565
$Li_6(H_2)_4$ iso_6	12	-4.8081	13	0.0488	4.8569
$Li_6(H_2)_4$ iso_7	12	-4.7713	13	0.0601	4.8314
$Li_6(H_2)_4$ iso_8	12	-4.7470	13	-0.2049	4.5421

Table S14. Pearson correlation coefficients (r) between energy components (E_{int}, E_{def} and $\Delta E_{adsTotal}$) and the structural/electronic descriptors for the $Li_6(H_2)_n$ global minima.

Energy Component	$r_{H–H}$	$d_{Li–H}$	$r_{Li–Li}$	RMSD	$\Delta d_{Li–H}$	μ (Site)
E_{int}	–0.55	0.05	0.95	0.40	–0.42	–0.18
E_{def}	0.29	–0.76	0.22	0.37	–0.79	0.34
$\Delta E_{adsTotal}$	–0.69	0.15	0.98	0.48	–0.39	–0.27

Table S15. Correlation Table: Superatom Stability vs. Aromaticity

Sistema (n)	NICS(0) (ppm)	Carga NNA (e)	Vol. NNA ($Bohr^3$)	Gap H-L (eV)	Status
Li_6	-13.29	-1.074	213.2	4.88	Base
$Li_6(H_2)_1$	-10.74	-1.072	212.8	4.89	Strongly Aromatic
$Li_6(H_2)_2$	-13.98	-1.059	210.4	5.04	Strongly Aromatic
$Li_6(H_2)_3$	-13.85	-1.057	211.1	5.04	Strongly Aromatic
$Li_6(H_2)_4$	-13.70	-1.055	211.6	5.05	Strongly Aromatic