Supplementary Information

The binary boron lithium clusters $B_{12}Li_n$ with n = 3 – 14: In search for hydrogen storage materials

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1. Assessments of the performance of different functionals for the search ofS stable binary boron lithium clusters.

The TPSSh[1] and PBE0[2] functionals in conjunction with the 6-311+G(d)[3,4] or def2-TZVP[5,6] basis sets were intensively used for searching the stable geometries and evaluating the relative energies between isomers of pure boron and boron doped clusters.[7–13] Recently, some authors proposed that the HSE06[14] or M06-2X[15] functionals could produce good geometries for boron based compounds.[16,17] To further confirm that calculations at the TPSSh/6-311+G(d) level provide us with enough accuracy compared to other high accuracy wavefunction levels, we consider three lowest-lying isomers of $B_{12}Li$ [18] (the **1A**, **1B**, and **1C** in Figure 1) to perform a benchmark test for these functionals and basis sets. The B3LYP,[19,20] M06,[15] wB97X[21] and wB97XD[22] functionals are also considered to ensure a greater diversity of approximations and approaches. Results of optimization calculations at the DFT/6-311+G(d) or DFT/def2-TZVP are then evaluated by performing single point electronic energy computations with the high accuracy coupled cluster

theory (U)CCSD(T) with the cc-pVTZ basis set. Obtained results are shown in Table S1 along with the root mean square (RMS) of energies differences. The TPSSh/6-311+G(d) level appears to give the most accurate results in all three isomers considered. The RSM = 0 value confirms it to be the most suitable theoretical level in the study of B_xLi_y clusters. It is also easy regconized that the 6-311+G(d) basis set gives better geometric optimization results than the def2-TZVP. The The HSE06/6-311+G(d) and PBE0/6-311+G(d) are two next best levels following by B3LYP/6-311+G(d). The remaining theoretical levels are not recommended in investigation of the geometry and energy of B_xLi_y clusters.

Table S1. (U)CCSD(T)/cc-pVTZ energies with respect to the lowest energy geometry of each species as optimized by each functional. Energies are in kcal/mol.

	1A	**1B**	**1C**	RMS
B3LYP/6-311+G(d)	0.47	0.53	0.51	0.50
HSE06/6-311+G(d)	0.32	0.39	0.37	0.36
HSE06/ def2-TZVP	0.69	0.86	0.79	0.78
M06/6-311+G(d)	1.33	1.21	1.18	1.24
M06-2X/6-311+G(d)	1.28	0.98	1.02	1.10
M06-2X/ def2-TZVP	1.69	1.55	1.60	1.61
PBE0/6-311+G(d)	0.35	0.40	0.38	0.37
PBE0/ def2-TZVP	0.69	0.84	0.77	0.77
TPSSh/6-311+G(d)	0.00	0.00	0.00	0.00
TPSSh/def2-TZVP	0.19	0.31	0.26	0.26
wB97X/6-311+G(d)	1.23	0.97	1.08	1.10
wB97XD/6-311+G(d)	1.00	0.72	0.71	0.82

Figure S1 presents the relative energies Δ_{21} and Δ_{31} of the isomer **1B** and **1C** with respect to the most stable isomer **1A** of the DFT and CCSD(T)/cc-pVTZ calculations. In the context that the structure cannot be optimized at the CCSD(T) level, we use single point CCSD(T) electronic energy from TPSSh/6-311+G(d) geometries as reference energies. The most serious error occurs for two levels B3LYP/6-311+G(d) and wB97XD/6-311+G(d): relative energies of the B3LYP is too small while that of wB97XD is too large, as compared to reference energies.

Results of the HSE06, PBE0, TPSSh functionals in conjunction with 6-311+G(d) basis set are better than those using def2-TZVP basis set. Finally, we would conclude that **the TPSSh/6-311+G(d) level is a adequate level to produce good geometries and to evaluate reliable relative energies of the B_xLi_y clusters.**

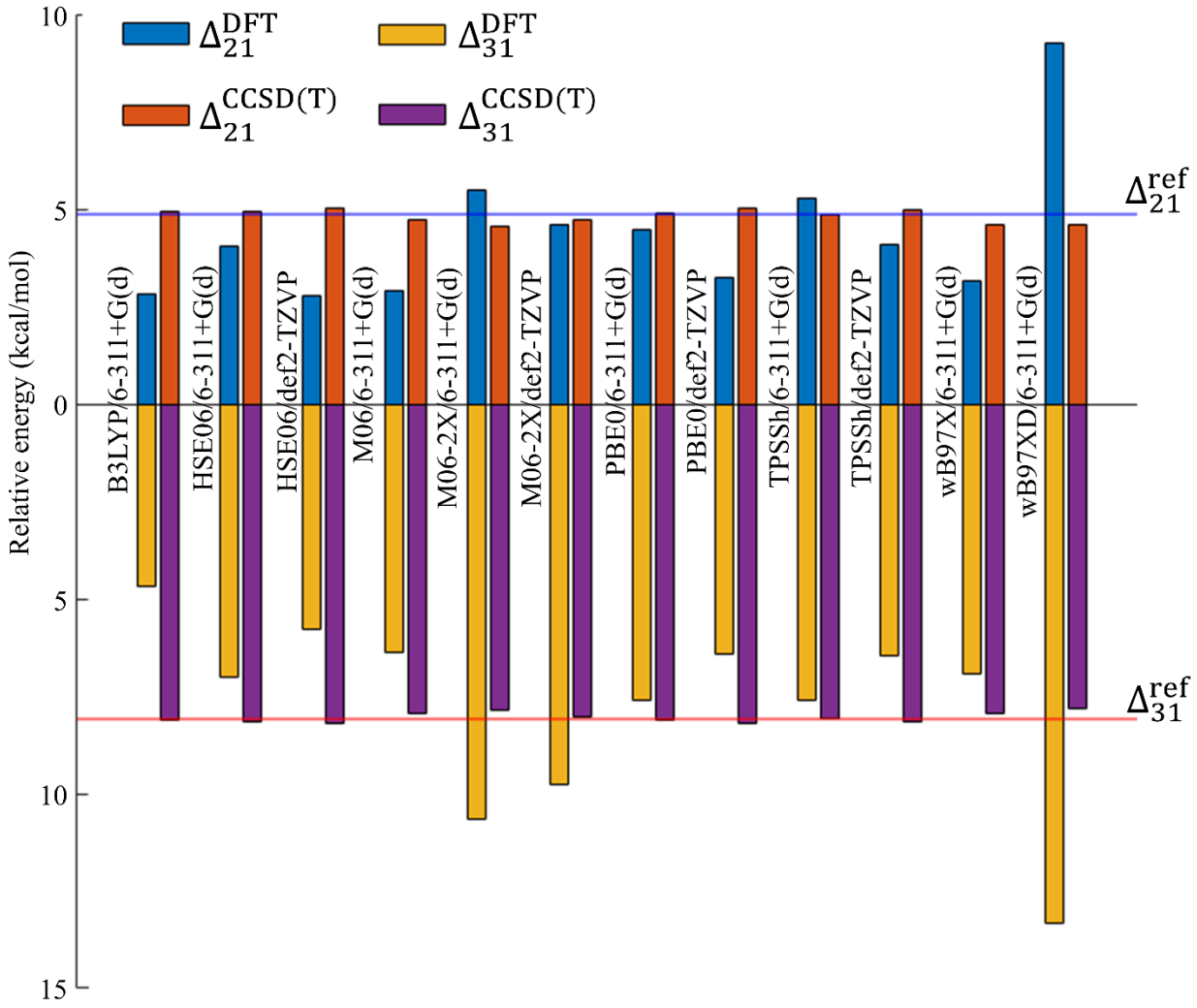

Figure S1. Relative energies Δ_{21} and Δ_{31} of isomers **1B** and **1C** with respect to the lowest-lying **1A** from DFT and CCSD(T)/cc-pVTZ calculations. The Δ_{21}^{ref} and Δ_{21}^{ref} lines are taken the CCSD(T)/cc-pVTZ energies at TPSSh/6-311+G(d) optimized geometries.

2. Average absorption energy survey with different functionals

The average adsorption energies (E_{abs}) of the **8A**-*m*H_2 systems with m = 1, 8, 16, 24, 32 and 40 determined using the TPSSh, M06, M06-2X, wB97X, and wB97XD functionals in conjunction with the 6-311++G(2d,2p)[3,4] basis set are shown in Table S2.

The TPSSh functional is not suitable for the study of hydrogen absorption because its E_{abs} values are significantly small as compared to results obtained from other functionals with m = 1, 8 and 16, and the **8A**-24H_2 complex is broken. The four commonly used functionals M06, M06-2X, wB97X and wB97XD in the hydrogen adsorption capacity survey give results quite close to each other, but with a better performance for the wB97XD and M06.

Table S2. Average absorption energy of the **8A**-*m*H_2 systems with m = 1; 8; 16; 24; 32; and 40 in different functionals in conjunction with 6-311++G(2d,2p) basis set.

	$1H_2$	$8H_2$	$16H_2$	$24H_2$	$32H_2$	$40H_2$
TPSSh	0.091	0.083	0.052	--	--	--
M06	0.141	0.129	0.117	0.110	0.110	0.096
M06-2X	0.128	0.112	0.096	0.086	0.080	0.069
wB97X	0.123	0.108	0.095	0.087	0.083	0.074
wB97XD	0.149	0.130	0.116	0.103	0.095	0.081

3. Cartesian coordinates of lower-lying isomers

Cartesian coordinates of some optimized structures computed at the TPSSh/6-311+G(d) level. The sum of bond orders (SBOs) and net atomic charges (NACs) of each atom are also given.

0A (B_{12})

Atom	X	Y	Z	SBOs	NACs
B	-1.60165900	1.82554200	-0.18402700	3.19	-0.07
B	1.60165900	1.82554200	-0.18402700	3.19	-0.07
B	-2.38179500	0.47430700	-0.18402700	3.19	-0.07
B	2.38179500	0.47430700	-0.18402700	3.19	-0.07
B	-0.78013600	-2.29984900	-0.18402700	3.19	-0.07

B	0.78013600	-2.29984900	-0.18402700	3.19	-0.07
B	-1.75673700	-1.01425300	-0.04377200	3.23	0.06
B	1.75673700	-1.01425300	-0.04377200	3.23	0.06
B	0.00000000	2.02850500	-0.04377200	3.23	0.06
B	-0.84393500	0.48724600	0.41182600	3.55	0.08
B	0.84393500	0.48724600	0.41182600	3.55	0.08
B	0.00000000	-0.97449200	0.41182600	3.55	0.08

1A ($B_{12}Li$)

Atom	X	Y	Z	SBOs	NACs
B	-0.17968600	2.32511300	-0.77140500	3.33	-0.13
B	-0.17968600	2.32511300	0.77140500	3.33	-0.13
B	-0.15230200	-0.45876100	-2.30339100	3.36	-0.12
B	-0.15230200	-0.45876100	2.30339100	3.36	-0.12
B	0.00546000	1.02607000	-1.71817100	3.43	-0.01
B	0.00546000	1.02607000	1.71817100	3.43	-0.01
B	-0.01297100	-2.14989300	0.00000000	3.45	-0.07
B	-0.14488200	-1.80585200	1.53383700	3.46	-0.14
B	-0.14488200	-1.80585200	-1.53383700	3.46	-0.14
B	0.67718500	-0.44673400	-0.84033500	3.57	0.01
B	0.67718500	-0.44673400	0.84033500	3.57	0.01
B	0.53000800	1.00368800	0.00000000	3.75	0.02
Li	-1.54764600	-0.22244600	0.00000000	0.35	0.82

2A ($B_{12}Li_2$)

Atom	X	Y	Z	SBOs	NACs
B	0.00000000	1.60580600	0.76820000	3.65	-0.13
B	1.39066900	0.80290300	0.76820000	3.65	-0.13
B	-1.39066900	0.80290300	0.76820000	3.65	-0.13
B	1.39066900	-0.80290300	0.76820000	3.65	-0.13
B	-1.39066900	-0.80290300	0.76820000	3.65	-0.13
B	0.00000000	-1.60580600	0.76820000	3.65	-0.13
B	-0.80290300	1.39066900	-0.76820000	3.65	-0.13
B	0.80290300	1.39066900	-0.76820000	3.65	-0.13
B	-1.60580600	0.00000000	-0.76820000	3.65	-0.13
B	1.60580600	0.00000000	-0.76820000	3.65	-0.13
B	-0.80290300	-1.39066900	-0.76820000	3.65	-0.13
B	0.80290300	-1.39066900	-0.76820000	3.65	-0.13
Li	0.00000000	0.00000000	-2.30391600	0.52	0.77
Li	0.00000000	0.00000000	2.30391600	0.52	0.77

3A ($B_{12}Li_3$)

Atom	X	Y	Z	SBOs	NACs
B	-0.10183700	-2.57871100	0.00000000	3.38	0.01
B	1.00496900	-1.12341800	0.00000000	3.45	0.08
B	0.03743600	-1.81313700	-1.34848800	3.58	-0.26
B	0.03743600	-1.81313700	1.34848800	3.58	-0.26
B	-0.19464500	2.42524100	-0.78209000	3.67	-0.15
B	-0.19464500	2.42524100	0.78209000	3.67	-0.15
B	0.20647200	1.26527000	-1.67986700	3.78	-0.41
B	0.20647200	1.26527000	1.67986700	3.78	-0.41
B	-0.56984600	0.86094100	0.00000000	3.87	-0.05
B	0.57202800	-0.29609000	-1.45080000	3.96	-0.21
B	0.57202800	-0.29609000	1.45080000	3.96	-0.21
B	-0.76227700	-0.84030800	0.00000000	4.06	-0.48
Li	-1.55668800	-0.17617300	-1.95252000	0.38	0.84
Li	-1.55668800	-0.17617300	1.95252000	0.38	0.84
Li	1.75739100	1.21722900	0.00000000	0.41	0.83

4A ($B_{12}Li_4$)

Atom	X	Y	Z	SBOs	NACs
B	-1.32940600	-1.00877800	-1.51268000	3.60	-0.20
B	-1.32940600	-1.00877800	1.51268000	3.60	-0.20
B	2.23294800	-0.57202300	0.00000000	3.61	-0.18
B	0.09004700	-0.65700000	-2.02751100	3.76	-0.24
B	0.09004700	-0.65700000	2.02751100	3.76	-0.24
B	1.51621400	-0.37633700	-1.37345700	3.81	-0.30
B	1.51621400	-0.37633700	1.37345700	3.81	-0.30
B	-1.77863900	-0.77102300	0.00000000	3.83	-0.24
B	1.11420300	0.77267200	0.00000000	3.88	-0.03
B	-0.75203700	0.49279300	-0.91729400	4.14	-0.14
B	-0.75203700	0.49279300	0.91729400	4.14	-0.14
B	-0.20828300	1.74698600	0.00000000	4.41	-1.16
Li	0.29871400	-1.92754100	0.00000000	0.36	0.86
Li	-2.38387800	1.66684000	0.00000000	0.38	0.84
Li	0.70102900	1.73204500	-1.97563000	0.42	0.83
Li	0.70102900	1.73204500	1.97563000	0.42	0.83

4E ($B_{12}Li_4$)

Atom	X	Y	Z	SBOs	NACs
B	0.00000000	1.85406700	-0.35538500	3.75	-0.20
B	1.60566900	-0.92703400	-0.35538500	3.76	-0.20
B	-1.60566900	-0.92703400	-0.35538500	3.76	-0.20
B	-1.07198800	-1.49657700	1.02110500	3.84	-0.45
B	-0.76008000	1.67665700	1.02110500	3.84	-0.45
B	1.83206800	-0.18008000	1.02110500	3.84	-0.45
B	-0.87470300	-0.36686000	-1.70269300	3.85	-0.30
B	0.75506200	-0.57408500	-1.70269300	3.85	-0.30
B	0.11964100	0.94094500	-1.70269300	3.85	-0.30
B	0.73299700	0.98678700	0.97153400	3.89	-0.12
B	0.48808400	-1.12818800	0.97153400	3.89	-0.12
B	-1.22108100	0.14140100	0.97153400	3.89	-0.12
Li	0.00000000	0.00000000	2.82640200	0.40	0.82
Li	-2.03102700	1.34092300	-0.83306900	0.46	0.81
Li	-0.14576000	-2.42938300	-0.83306900	0.46	0.81
Li	2.17678700	1.08845900	-0.83306900	0.46	0.80

5A ($B_{12}Li_5$)

Atom	X	Y	Z	SBOs	NACs
B	-0.84892200	-2.02449100	-0.25792600	3.76	-0.18
B	2.11098500	-1.37640300	0.12142900	3.78	-0.25
B	-2.14547700	-1.20804500	0.07517800	3.82	-0.47
B	0.72093900	-2.05073000	0.03407900	3.84	-0.33
B	-0.41517700	0.86696000	1.06415000	3.88	-0.60
B	-1.44094200	1.58261900	-0.09934700	3.89	-0.55
B	2.51940600	0.08330400	-0.27469700	3.92	-0.32
B	-2.09757600	0.29267400	0.64467800	3.93	-0.21
B	1.65278200	1.31081900	-0.65436500	3.94	-0.56
B	0.01953400	1.23668400	-0.86038400	4.06	-0.25
B	-0.79105200	-0.20600200	-0.41770100	4.12	-0.07
B	0.83959400	-0.12786200	0.28714800	4.14	-0.11
Li	-2.79035000	0.51044400	-1.39353500	0.39	0.83
Li	1.02397500	-0.71294200	-1.84711600	0.40	0.84
Li	-0.58764400	-1.19484700	1.79613600	0.43	0.83
Li	0.27896500	2.98954400	0.29775100	0.55	0.72
Li	1.86822900	1.10859000	1.70969800	0.58	0.69

6A ($B_{12}Li_6$)

Atom	X	Y	Z	SBOs	NACs
B	2.56887300	0.48745100	-0.16765300	3.84	-0.20
B	0.95503300	0.06120700	0.35671600	3.87	0.04
B	-2.36761200	0.55685500	0.38032000	3.88	-0.36
B	2.23778600	-0.99434600	-0.43799900	3.91	-0.46
B	1.61836700	1.72641100	-0.01133400	3.97	-0.47
B	-1.54386800	1.83387000	0.01685700	4.00	-0.53
B	-0.89306900	0.26462700	-0.45715300	4.06	0.05
B	-0.71914400	-1.36778200	-0.89359700	4.14	-0.75
B	0.85453100	-1.76566100	-0.36232000	4.18	-0.33
B	-1.79674500	-0.96105800	0.46318600	4.24	-0.47
B	-0.15711600	-1.15169300	0.93858400	4.30	-0.78
B	0.04878300	1.70287100	-0.24728100	4.69	-0.59
Li	0.93858900	0.20163700	-1.87342500	0.39	0.85
Li	0.11118500	3.60689700	0.26375600	0.44	0.79
Li	-2.65706100	-0.66186400	-1.50866200	0.45	0.81
Li	-0.66147800	0.79124700	1.81356800	0.46	0.83
Li	1.83953100	-1.55713400	1.64539600	0.50	0.78
Li	-0.91379800	-3.03537100	0.36215700	0.50	0.80

7A ($B_{12}Li_7$)

Atom	X	Y	Z	SBOs	NACs
B	-2.64822000	-0.10028500	-0.04285600	3.77	-0.31
B	0.71779200	-2.04591800	-0.34337200	3.78	-0.22
B	-0.78361300	-2.19489600	0.14767900	3.79	-0.28
B	-2.20361300	-1.56082700	0.26787900	3.80	-0.29
B	-0.99076700	-0.32990000	0.39173300	4.05	-0.06
B	2.01475700	-1.16741500	-0.42190200	4.08	-0.51
B	0.61195100	-0.15436800	-0.47309100	4.09	0.03
B	-0.28037800	1.14852200	-1.16781100	4.12	-0.67
B	-1.74806000	1.20718300	-0.27539600	4.17	-0.45
B	2.21649400	0.36011500	-0.05949800	4.24	-0.63
B	1.11854000	1.55930300	-0.25971200	4.28	-0.53
B	-0.27560900	1.21566000	0.75325100	4.34	-0.82
Li	1.61142800	0.64296000	-2.21715000	0.41	0.84
Li	-1.21549900	-0.89288400	-1.74970300	0.44	0.82
Li	-2.08881800	0.94742700	1.88903700	0.49	0.78
Li	-0.51356600	3.05729700	-0.25463000	0.49	0.80
Li	3.49434500	-0.93432700	1.27734800	0.77	0.46
Li	0.74446100	-0.96955700	1.66087700	0.83	0.57

Li	1.71885900	1.58712800	1.86604800	0.90	0.47

8A ($B_{12}Li_8$)

Atom	X	Y	Z	SBOs	NACs
B	2.38813300	0.00000000	-0.33387000	4.01	-0.97
B	-2.38813300	0.00000000	-0.33387000	4.01	-0.97
B	-0.83607500	0.00000000	-1.17241500	4.02	-0.06
B	0.83607500	0.00000000	-1.17241500	4.02	-0.06
B	-1.29090000	-1.04274100	0.36441300	4.14	-0.24
B	1.29090000	-1.04274100	0.36441300	4.14	-0.24
B	-1.29090000	1.04274100	0.36441300	4.14	-0.24
B	1.29090000	1.04274100	0.36441300	4.14	-0.24
B	0.00000000	-1.48279800	-0.73350400	4.21	-0.82
B	0.00000000	1.48279800	-0.73350400	4.21	-0.82
B	0.00000000	-0.83592400	1.53401100	4.23	-0.74
B	0.00000000	0.83592400	1.53401100	4.23	-0.74
Li	1.90890700	0.00000000	2.15835500	0.44	0.84
Li	-1.90890700	0.00000000	2.15835500	0.44	0.84
Li	-2.08130100	-1.76207800	-1.54227800	0.56	0.75
Li	2.08130100	-1.76207800	-1.54227800	0.56	0.75
Li	-2.08130100	1.76207800	-1.54227800	0.56	0.75
Li	2.08130100	1.76207800	-1.54227800	0.56	0.75
Li	0.00000000	2.81901300	0.88778800	0.60	0.74
Li	0.00000000	-2.81901300	0.88778800	0.60	0.74

9A ($B_{12}Li_9$)

Atom	X	Y	Z	SBOs	NACs
B	2.48329500	0.00000000	0.10310600	3.91	-0.94
B	-2.48329500	0.00000000	0.10310600	3.91	-0.94
B	-1.31532500	-1.02610400	-0.46933300	4.11	-0.21
B	-1.31532500	1.02610400	-0.46933300	4.11	-0.21
B	1.31532500	-1.02610400	-0.46933300	4.11	-0.21
B	1.31532500	1.02610400	-0.46933300	4.11	-0.21
B	0.00000000	-1.46762800	0.66615900	4.17	-0.76
B	0.00000000	1.46762800	0.66615900	4.17	-0.76
B	0.00000000	-0.83988400	-1.57899400	4.23	-0.73
B	0.00000000	0.83988400	-1.57899400	4.23	-0.73
B	-0.89776600	0.00000000	1.06889200	4.36	-0.37
B	0.89776600	0.00000000	1.06889200	4.36	-0.37
Li	-1.86842500	0.00000000	-2.28877200	0.45	0.84

Li	1.86842500	0.00000000	-2.28877200	0.45	0.84
Li	0.00000000	-2.82587000	-0.93992300	0.60	0.73
Li	0.00000000	2.82587000	-0.93992300	0.60	0.73
Li	-2.19544000	-1.67250000	1.43293800	0.64	0.70
Li	2.19544000	-1.67250000	1.43293800	0.64	0.70
Li	2.19544000	1.67250000	1.43293800	0.65	0.70
Li	-2.19544000	1.67250000	1.43293800	0.65	0.70
Li	0.00000000	0.00000000	2.99065200	0.78	0.52

10A ($B_{12}Li_{10}$)

Atom	X	Y	Z	SBOs	NACs
B	-1.28522900	-0.35876700	-0.92800300	3.99	-0.30
B	-1.28522900	-0.35876700	0.92800300	3.99	-0.30
B	0.06650200	-1.75993500	0.00000000	4.03	-0.03
B	1.66018400	-0.69242900	0.00000000	4.07	-1.03
B	-0.55179100	-1.68658700	-1.57411400	4.13	-1.01
B	-0.55179100	-1.68658700	1.57411400	4.13	-1.01
B	0.82697500	0.77209600	0.00000000	4.18	0.05
B	0.49532400	-0.35862500	1.39845800	4.41	-0.32
B	0.49532400	-0.35862500	-1.39845800	4.41	-0.32
B	-0.31395500	1.14501300	-1.34483500	4.45	-0.83
B	-0.31395500	1.14501300	1.34483500	4.45	-0.83
B	0.11752800	2.25162300	0.00000000	4.53	-1.16
Li	-1.98333300	-2.31268700	0.00000000	0.45	0.84
Li	-2.02673000	1.46206500	0.00000000	0.51	0.81
Li	2.06374700	1.10888600	-1.58479700	0.61	0.70
Li	2.06374700	1.10888600	1.58479700	0.62	0.70
Li	-0.78558100	-0.10363500	-3.06660600	0.62	0.73
Li	-0.78558100	-0.10363500	3.06660600	0.62	0.73
Li	1.52742700	-2.24275200	-1.58641800	0.63	0.72
Li	1.52742700	-2.24275200	1.58641800	0.63	0.71
Li	-0.26713400	3.28495800	-1.77081200	0.79	0.57
Li	-0.26713400	3.28495800	1.77081200	0.79	0.57

11A ($B_{12}Li_{11}$)

Atom	X	Y	Z	SBOs	NACs
B	0.68237600	0.85708000	0.00000000	4.00	0.06
B	-1.27453400	-0.65549600	-0.92531000	4.00	-0.31
B	-1.27453400	-0.65549600	0.92531000	4.00	-0.31
B	0.23988700	-1.80246800	0.00000000	4.04	-0.02
B	-0.35156400	-1.84667600	-1.58499400	4.09	-1.01

B	-0.35156400	-1.84667600	1.58499400	4.09	-1.01
B	1.67092700	-0.53060900	0.00000000	4.10	-1.03
B	-0.55790500	0.98254300	1.32049000	4.36	-0.74
B	-0.55790500	0.98254300	-1.32049000	4.36	-0.74
B	0.47899100	-0.36609800	1.37444900	4.36	-0.29
B	0.47899100	-0.36609800	-1.37444900	4.36	-0.29
B	-0.39670200	2.13658900	0.00000000	4.42	-1.05
Li	-1.67889200	-2.70274800	0.00000000	0.42	0.85
Li	-2.34728200	0.99888600	0.00000000	0.48	0.82
Li	1.77761400	-2.09100600	-1.58380100	0.60	0.73
Li	1.77761400	-2.09100600	1.58380100	0.61	0.72
Li	-0.79583500	-0.30920900	-3.07367300	0.62	0.72
Li	-0.79583500	-0.30920900	3.07367300	0.62	0.72
Li	-0.72878300	3.05732200	-1.90285400	0.81	0.53
Li	-0.72878300	3.05732200	1.90285400	0.81	0.53
Li	2.06563300	1.09761300	-1.62925600	0.84	0.54
Li	2.06563300	1.09761300	1.62925600	0.84	0.54
Li	1.41147900	3.37919100	0.00000000	1.22	0.08

12A ($B_{12}Li_{12}$)

Atom	X	Y	Z	SBOs	NACs
B	0.53342500	0.85024600	0.00000000	3.89	0.12
B	-1.31262900	-0.78379200	-0.92112900	3.98	-0.29
B	-1.31262900	-0.78379200	0.92112900	3.98	-0.29
B	0.29066500	-1.81877800	0.00000000	4.02	-0.02
B	-0.30585300	-1.91183600	-1.58839200	4.08	-1.03
B	-0.30585300	-1.91183600	1.58839200	4.08	-1.03
B	1.61286500	-0.45479100	0.00000000	4.15	-0.97
B	0.39947700	-0.37544500	1.36768200	4.34	-0.27
B	0.39947700	-0.37544500	-1.36768200	4.34	-0.27
B	-0.72772600	0.89626300	1.32519900	4.37	-0.79
B	-0.72772600	0.89626300	-1.32519900	4.37	-0.79
B	-0.59808900	2.07413700	0.00000000	4.40	-1.06
Li	-1.54255500	-2.87385900	0.00000000	0.43	0.85
Li	-2.49461900	0.80032600	0.00000000	0.47	0.82
Li	1.84290800	-1.98531400	-1.61760300	0.60	0.72
Li	1.84290800	-1.98531400	1.61760300	0.60	0.72
Li	-0.86272600	-0.41258100	-3.07911100	0.63	0.71
Li	-0.86272600	-0.41258100	3.07911100	0.63	0.71
Li	-1.06078100	2.99471400	-1.87114600	0.81	0.53
Li	-1.06078100	2.99471400	1.87114600	0.81	0.53
Li	1.49005500	1.40100900	-1.91905600	1.02	0.42
Li	1.49005500	1.40100900	1.91905600	1.03	0.42

Li	3.41667800	0.84769500	0.00000000	1.08	0.18
Li	1.22590800	3.39485700	0.00000000	1.27	0.07

13A ($B_{12}Li_{13}$)

Atom	X	Y	Z	SBOs	NACs
B	-0.06751300	-0.62170500	0.29160500	3.96	-0.23
B	-0.84377400	-2.11164000	-0.40490600	4.02	-0.36
B	-1.45733800	0.50347400	0.30941600	4.12	-0.16
B	0.66188100	-2.26122400	-0.16547200	4.15	-0.54
B	1.43975200	0.29295000	0.31580200	4.17	-0.17
B	2.09534500	-1.52052100	-0.19867400	4.17	-0.31
B	-2.20141100	-1.25015800	-0.40600400	4.18	-0.34
B	3.01579500	-0.26389900	-0.06019000	4.27	-1.32
B	-3.06199800	0.01520500	-0.07451500	4.29	-1.36
B	0.05757200	0.88306300	-0.65720000	4.37	-0.54
B	-0.77365800	2.11897300	0.29046000	4.50	-1.07
B	0.95187700	2.04307600	0.30813400	4.59	-1.20
Li	4.29782200	-1.52495500	-0.98024300	0.54	0.74
Li	-4.54171200	-1.18459800	-0.71996400	0.55	0.73
Li	3.00365000	1.70776400	0.95968500	0.72	0.66
Li	-2.93841300	2.10653600	0.44412800	0.74	0.66
Li	0.18894800	3.87398300	0.99408200	0.74	0.62
Li	0.67220500	-0.90310200	-1.88784700	0.75	0.62
Li	-1.83988000	0.60234100	-1.86632200	0.76	0.62
Li	-0.00626600	0.96156500	1.95939700	0.83	0.60
Li	-0.43143500	-3.67008700	1.24938300	0.86	0.34
Li	-0.01252100	2.90318100	-1.59540000	0.88	0.52
Li	2.27901100	1.34143500	-1.44119400	0.89	0.56
Li	1.42615300	-1.40434400	1.88321600	0.92	0.47
Li	-1.79177800	-1.18904300	1.75365400	0.98	0.45

14A ($B_{12}Li_{14}$)

Atom	X	Y	Z	SBOs	NACs
B	-0.17465500	0.17098500	0.98572200	3.82	0.30
B	-0.17465500	0.17098500	-0.98572200	3.82	0.30
B	0.69158800	1.40712200	0.00000000	4.24	-1.06
B	-1.82138500	-0.06846200	1.52778200	4.37	-0.89
B	-1.82138500	-0.06846200	-1.52778200	4.37	-0.89
B	-1.35859600	-0.73352700	0.00000000	4.39	-0.71
B	0.94979800	-0.60276500	2.12172300	4.47	-0.99
B	0.94979800	-0.60276500	-2.12172300	4.47	-0.99

B	1.66833100	0.23879200	0.86787600	4.57	-0.59
B	1.66833100	0.23879200	-0.86787600	4.57	-0.59
B	-0.58911200	0.03186900	2.68161000	4.64	-1.08
B	-0.58911200	0.03186900	-2.68161000	4.64	-1.08
Li	0.68449800	1.79444200	-2.19088400	0.66	0.71
Li	0.68449800	1.79444200	2.19088400	0.66	0.71
Li	-0.87550000	-2.05091100	-1.79732800	0.70	0.67
Li	-0.87550000	-2.05091100	1.79732800	0.70	0.67
Li	0.60177800	-0.60871100	-4.26965200	0.72	0.61
Li	0.60177800	-0.60871100	4.26965200	0.73	0.61
Li	-1.52261200	1.73378500	0.00000000	0.75	0.65
Li	-2.42682400	0.82140800	-3.34024900	0.80	0.57
Li	-2.42682400	0.82140800	3.34024900	0.81	0.57
Li	-3.43090500	-0.19601500	0.00000000	0.86	0.55
Li	3.08349700	-0.97451000	-1.84784200	0.89	0.46
Li	3.08349700	-0.97451000	1.84784200	0.90	0.46
Li	2.87308300	1.84804500	0.00000000	0.90	0.49
Li	0.94729400	-1.70663600	0.00000000	0.93	0.54

14C ($B_{12}Li_{14}$)

Atom	X	Y	Z	SBOs	NACs
B	1.01454500	0.16578600	-1.37795000	4.18	-0.52
B	-1.01454500	-0.16578600	1.37795000	4.18	-0.52
B	-0.65090800	0.79578900	-1.37810000	4.18	-0.52
B	0.65090800	-0.79578900	1.37810000	4.18	-0.52
B	0.36363800	0.96157500	1.37794900	4.18	-0.52
B	-0.36363800	-0.96157500	-1.37794900	4.18	-0.52
B	-1.07016900	1.30850400	0.27419700	4.20	-0.52
B	1.07016900	-1.30850400	-0.27419700	4.20	-0.52
B	0.59799800	1.58103000	-0.27419900	4.20	-0.52
B	-0.59799800	-1.58103000	0.27419900	4.20	-0.52
B	1.66814100	0.27259400	0.27411300	4.20	-0.52
B	-1.66814100	-0.27259400	-0.27411300	4.20	-0.52
Li	-0.00084900	-0.00124400	-3.32146200	0.80	0.55
Li	0.00084900	0.00124400	3.32146200	0.80	0.55
Li	-2.24354800	-2.01180600	-1.42444500	0.95	0.43
Li	-2.41687300	-1.79955100	1.42414200	0.95	0.43
Li	0.34883700	-2.99374700	-1.42247000	0.95	0.43
Li	-2.86488900	0.93568500	1.42274500	0.95	0.43
Li	0.62312300	-2.94871000	1.42278100	0.95	0.43
Li	-2.76741100	1.19247400	-1.42474600	0.95	0.43
Li	2.86488900	-0.93568500	-1.42274500	0.95	0.43
Li	-0.34883700	2.99374700	1.42247000	0.95	0.43
Li	2.76741100	-1.19247400	1.42474600	0.95	0.43

Li	2.41687300	1.79955100	-1.42414200	0.95	0.43
Li	-0.62312300	2.94871000	-1.42278100	0.95	0.43
Li	2.24354800	2.01180600	1.42444500	0.95	0.43

14C-T_h ($B_{12}Li_{14}$)

Atom	X	Y	Z	SBOs	NACs
B	0.93436000	1.43657000	0.00000000	4.19	-0.52
B	1.43657000	0.00000000	0.93436000	4.19	-0.52
B	0.00000000	0.93436000	1.43657000	4.19	-0.52
B	1.43657000	0.00000000	-0.93436000	4.19	-0.52
B	0.00000000	-0.93436000	1.43657000	4.19	-0.52
B	-0.93436000	1.43657000	0.00000000	4.19	-0.52
B	0.93436000	-1.43657000	0.00000000	4.19	-0.52
B	0.00000000	0.93436000	-1.43657000	4.19	-0.52
B	-1.43657000	0.00000000	0.93436000	4.19	-0.52
B	-1.43657000	0.00000000	-0.93436000	4.19	-0.52
B	-0.93436000	-1.43657000	0.00000000	4.19	-0.52
B	0.00000000	-0.93436000	-1.43657000	4.19	-0.52
Li	-1.91491900	-1.91491900	-1.91491900	0.91	0.47
Li	1.91491900	-1.91491900	-1.91491900	0.91	0.47
Li	-1.91491900	-1.91491900	1.91491900	0.91	0.47
Li	-1.91491900	1.91491900	-1.91491900	0.91	0.47
Li	1.91491900	1.91491900	-1.91491900	0.91	0.47
Li	-1.91491900	1.91491900	1.91491900	0.91	0.47
Li	1.91491900	-1.91491900	1.91491900	0.91	0.47
Li	1.91491900	1.91491900	1.91491900	0.91	0.47
Li	-3.36624400	0.00000000	0.00000000	0.94	0.41
Li	0.00000000	0.00000000	-3.36624400	0.94	0.41
Li	0.00000000	-3.36624400	0.00000000	0.94	0.41
Li	0.00000000	0.00000000	3.36624400	0.94	0.41
Li	0.00000000	3.36624400	0.00000000	0.94	0.41
Li	3.36624400	0.00000000	0.00000000	0.94	0.41

3. Figures

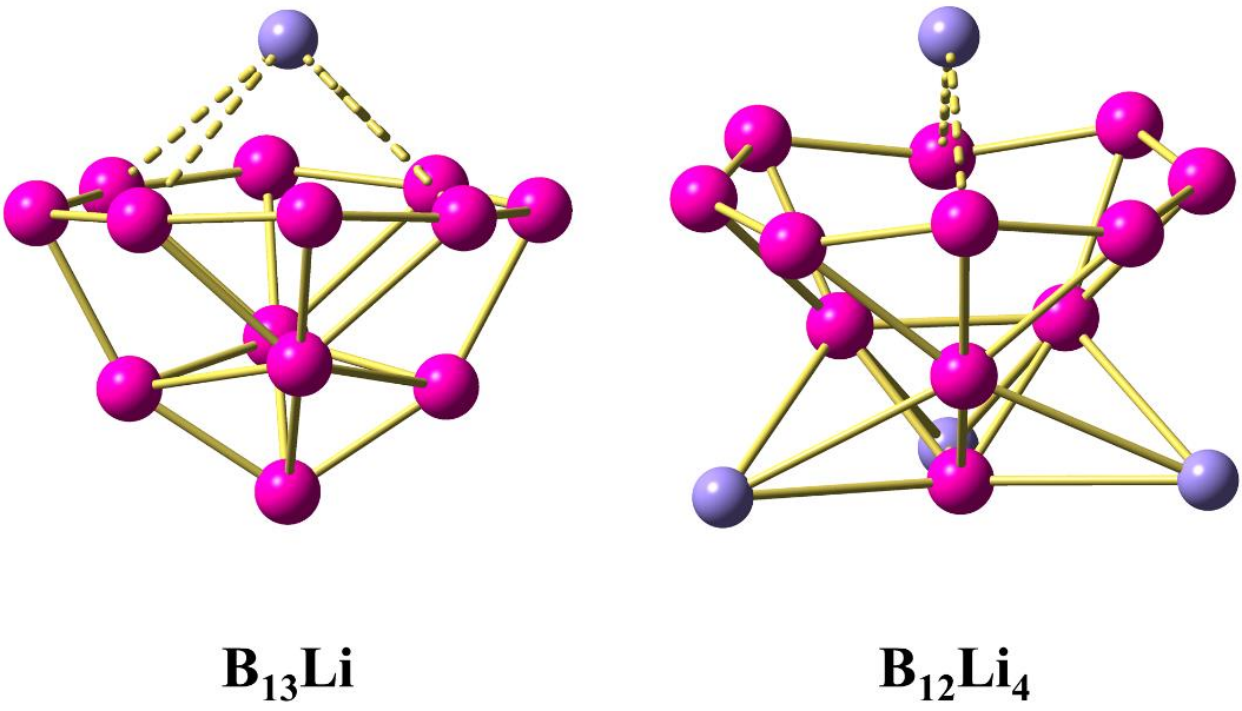

Figure S2. The lowest-energy structures of the isoelectronic $B_{13}Li$ and $B_{12}Li_4$.

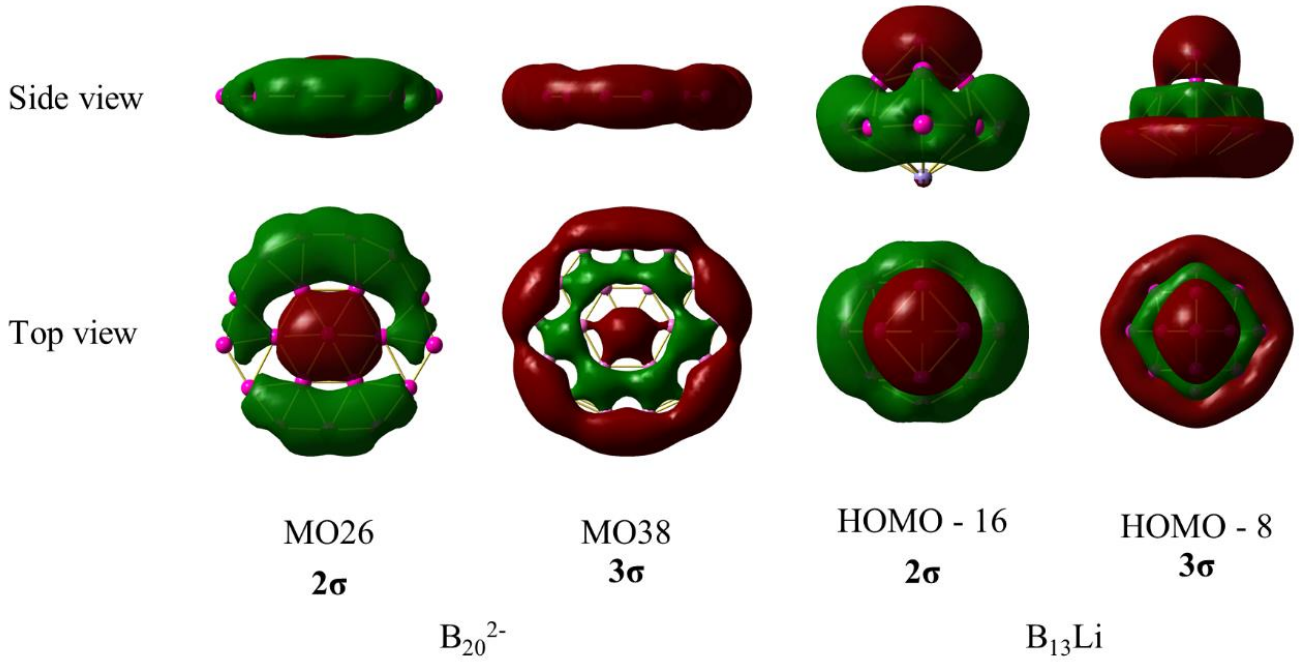

Figure S3. The 2σ and 3σ-orbitals of B_{20}^{2-} and $B_{13}Li$ under the top view and the side view.

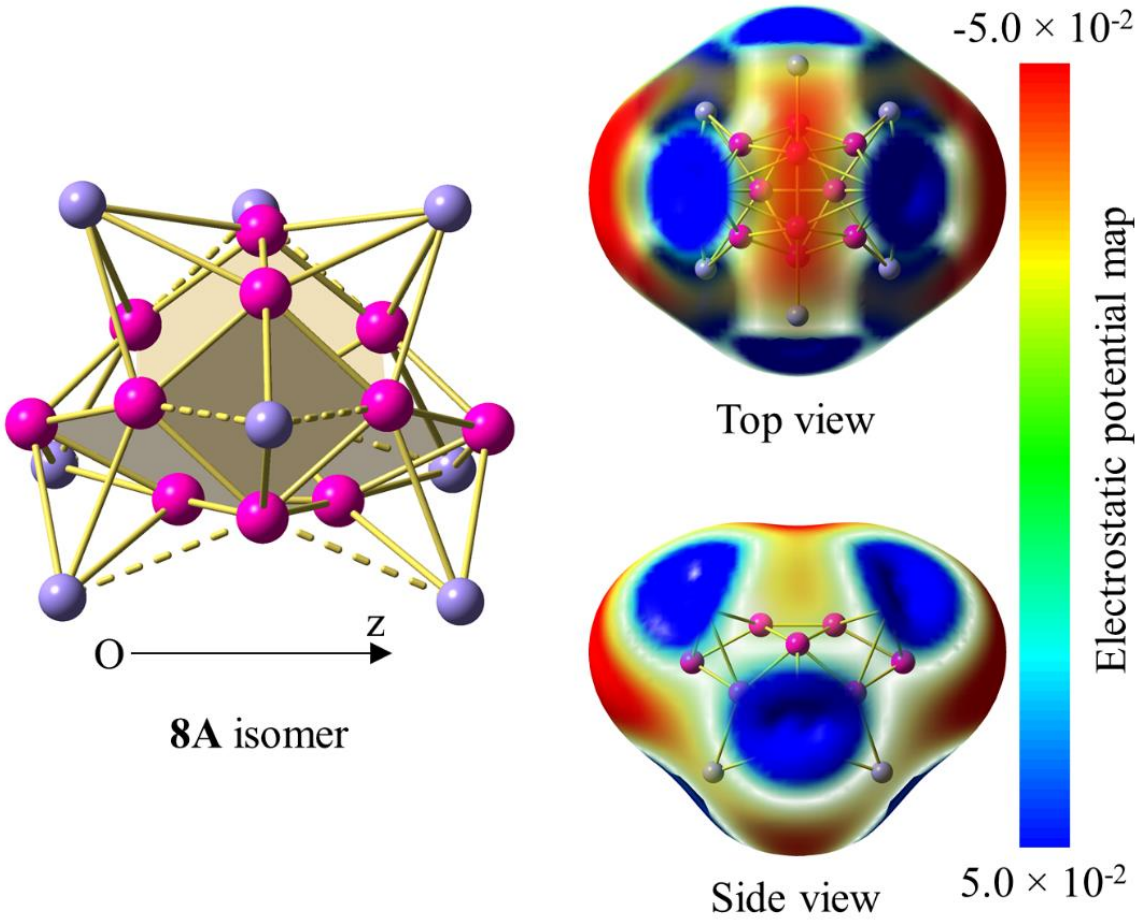

Figure S4. $B_{12}Li_8$ **8A** and its electrostatic potential map on the 0.001 electron/bohr^3 isodensity surface.

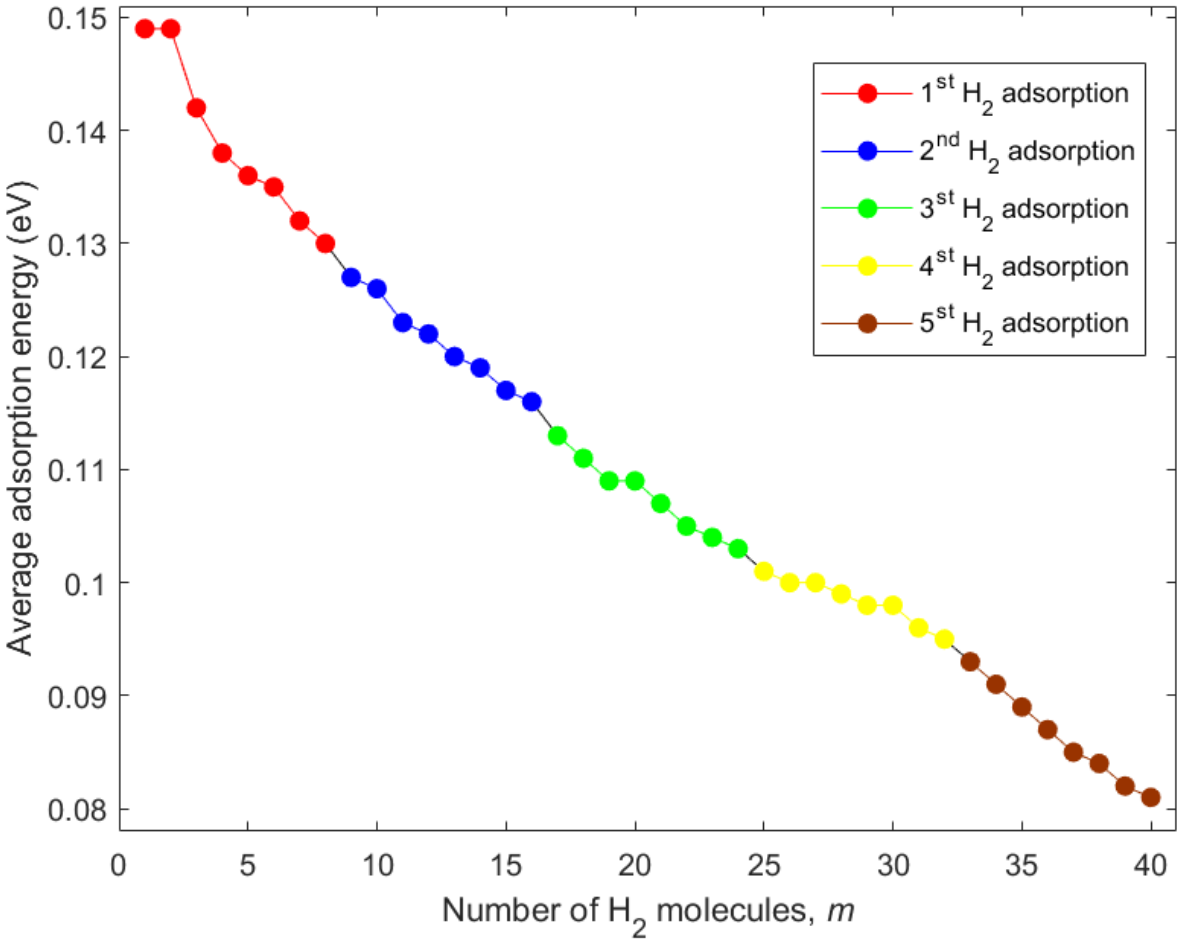

Figure S5. Average adsorption energies (E_{abs}, eV) per H_2 molecule of $B_{12}Li_8$-mH_2 calculated at the wB97XD/6-311+G(2d,2p) level.

References

1 V. N. Staroverov, G. E. Scuseria, J. Tao and J. P. Perdew, *J. Chem. Phys.*, 2003, **119**, 12129–12137.

2 C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158–6170.

3 R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650–654.

4 T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294–301.

5 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297.

6 F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057.

7 L. Cheng, *J. Chem. Phys.*, 2012, **136**, 104301.

8 Q. Chen, G.-F. Wei, W.-J. Tian, H. Bai, Z.-P. Liu, H.-J. Zhai and S.-D. Li, *Phys. Chem. Chem. Phys.*, 2014, **16**, 18282.

9 H. T. Pham and M. T. Nguyen, *Phys. Chem. Chem. Phys.*, 2015, **17**, 17335–17345.

10 D. T. T. Mai, L. V. Duong, M. P. Pham-Ho and M. T. Nguyen, *J. Phys. Chem. C*, 2020, **124**, 6770–6783.

11 T. B. Tai and M. T. Nguyen, *Nanoscale*, 2015, **7**, 3316–3317.

12 C. Li, Y. Cui, J. Li, J. Guo, L. Cheng, B. Ren and Y. Yuan, *Mol. Phys.*, 2021, e1910744.

13 L. Pei, M. Yan, X.-Y. Zhao, Y.-W. Mu, H.-G. Lu, Y.-B. Wu and S.-D. Li, *RSC Adv.*, 2020, **10**, 10129–10133.

14 A. V. Krukau, O. A. Vydrov, A. F. Izmaylov and G. E. Scuseria, *J. Chem. Phys.*, 2006, **125**, 224106.

15 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215–241.

16 E. N. Koukaras, *Phys. Chem. Chem. Phys.*, 2018, **20**, 18556–18570.

17 L. Sai, X. Wu, N. Gao, J. Zhao and R. B. King, *Nanoscale*, 2017, **9**, 13905–13909.

18 X. Dong, S. Jalife, A. Vásquez-Espinal, E. Ravell, S. Pan, J. L. Cabellos, W. Y. Liang, Z. H. Cui and G. Merino, *Angew. Chem. Int. Ed.*, 2018, **57**, 4627–4631.

19 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648–5652.

20 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785–789.

21 J.-D. Chai and M. Head-Gordon, *J. Chem. Phys.*, 2008, **128**, 084106.

22 J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615.