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

Supplementary Information

for

The teetotum cluster Li_2FeB_{14} and its possible use for constructing boron nanowires

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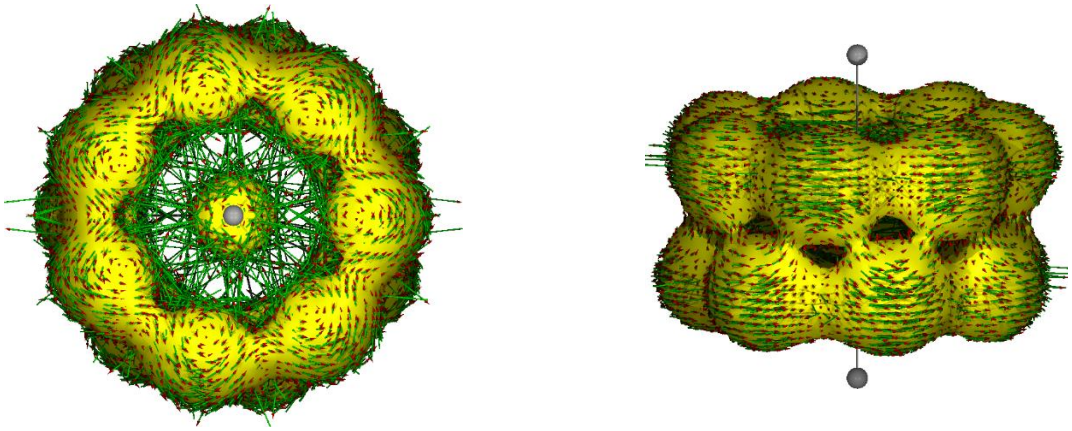
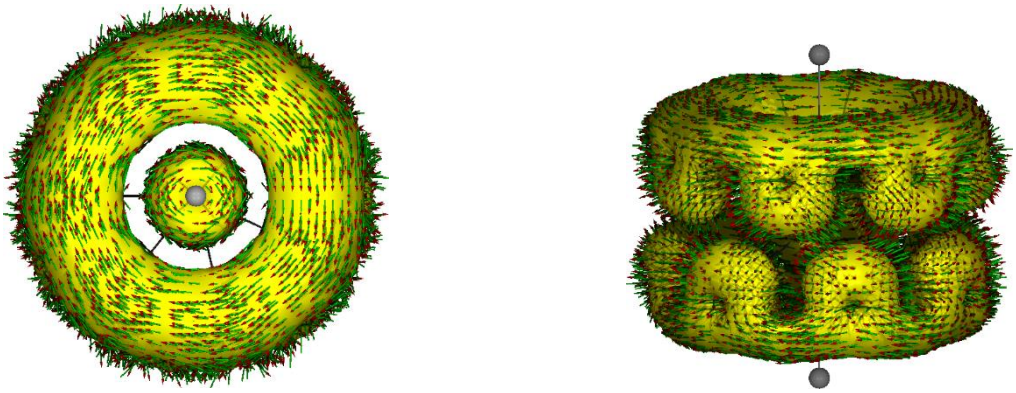


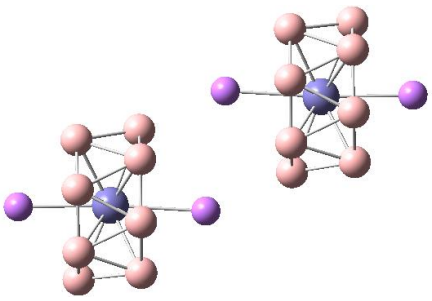
a) Localized

b) Tangential (σ)

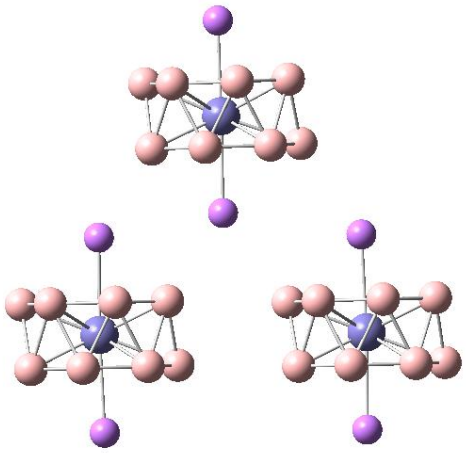


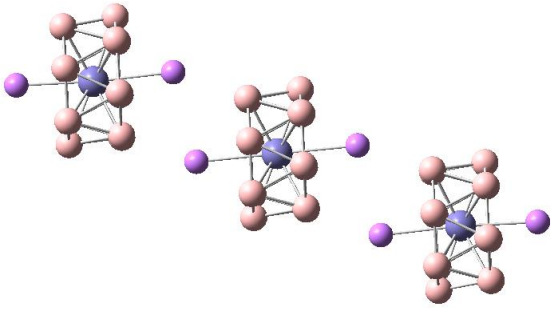
c) Radial (π)

Figure S1. AICD isosurface (isovalue = 0.05) of three valence MOs sets of $B_{14}FeLi_2$ on the view from Li-Fe-Li axis (Oz axis) including a) localized set, b) tangential set and c) radial set. The external magnetic field vector is placed along the Oz axis with the direction out of the paper plane (Z+). The clockwise current density vectors are plotted on the AICD isosurface are highlighted by the arrows with red glow while the anti-clockwise current density vectors ones are highlighted by the arrows with orange glow. The right figures are the view of the left figures after an 80º rotation of Ox axis.

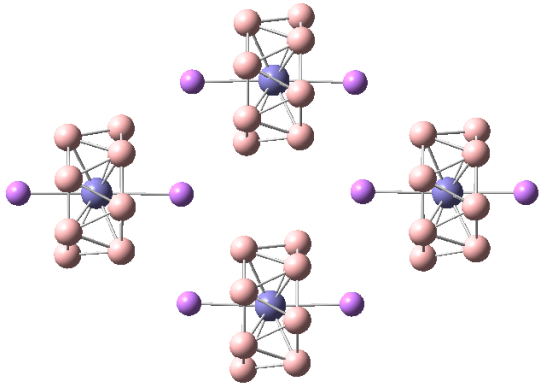


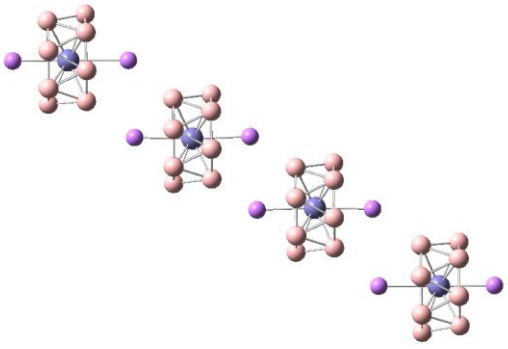
Dimer





Trimer





Tetramer

Fig. S2. Dimeric, trimeric and tetrameric forms of Li_2FeB_{14}.

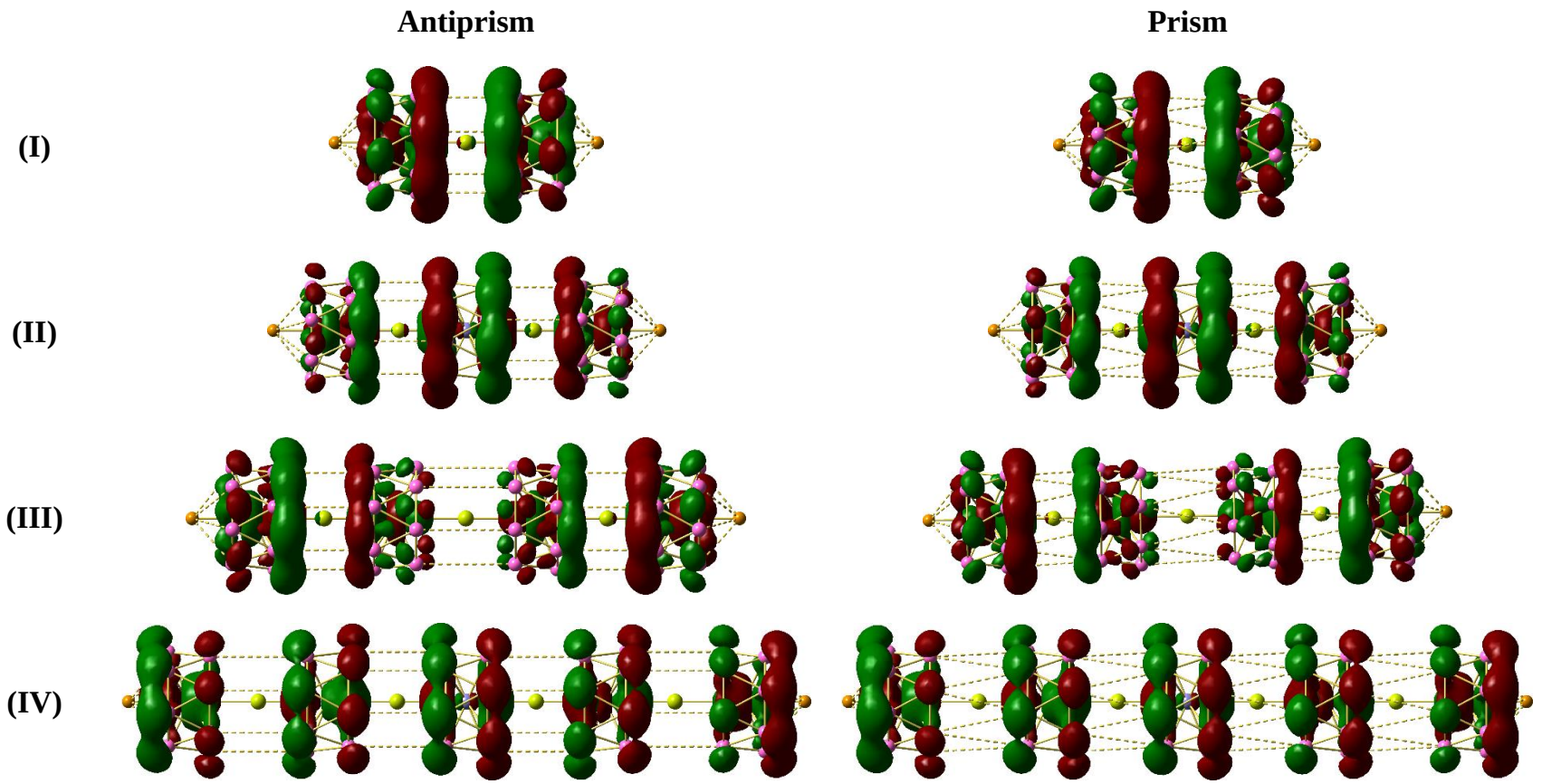
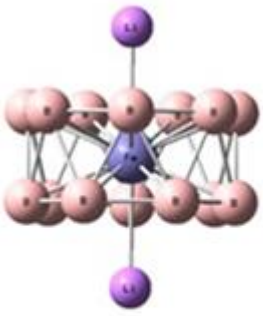


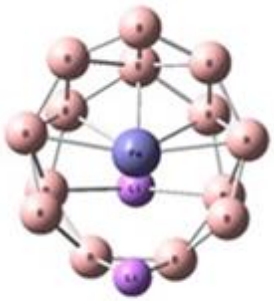
Figure S3. The HOMO of (**I**) $B_{28}Fe_2Li_2Mg$, (**II**) $B_{42}Fe_3Li_2Mg_2$, (**III**) $B_{56}Fe_4Li_2Mg_3$, and (**IV**) $B_{70}Fe_4Mg_4Li_2$ nanowires in antiprism and prism forms.



D_{7d}-$^1A_{1g}$

E+ZPE= -1626.819675 au

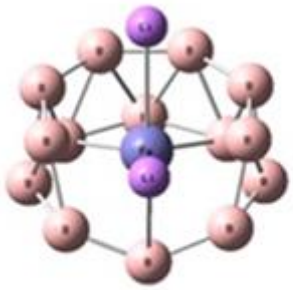
B	0.00000000	1.88226400	0.79991300
B	-1.47161300	1.17357200	0.79991300
B	-1.83507200	-0.41884300	0.79991300
B	-0.81668400	-1.69586100	0.79991300
B	0.81668400	-1.69586100	0.79991300
B	1.83507200	-0.41884300	0.79991300
B	1.47161300	1.17357200	0.79991300
B	0.81668400	1.69586100	-0.79991300
B	-0.81668400	1.69586100	-0.79991300
B	-1.83507200	0.41884300	-0.79991300
B	-1.47161300	-1.17357200	-0.79991300
B	0.00000000	-1.88226400	-0.79991300
B	1.47161300	-1.17357200	-0.79991300
B	1.83507200	0.41884300	-0.79991300
Fe	0.00000000	0.00000000	0.00000000
Li	0.00000000	0.00000000	-2.32041200
Li	0.00000000	0.00000000	2.32041200



C_s-$^1A'$

E+ZPE = -1626.804160 au

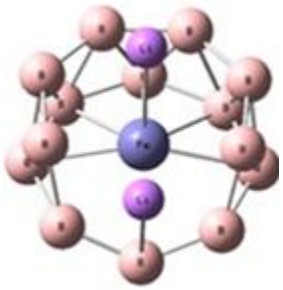
B	1.07303500	-0.83895400	1.36710900
B	-0.41616500	-0.28660400	2.11843600
B	-0.71347400	1.23762400	1.78837200
B	0.78240100	-1.70838300	0.00000000
B	-0.91597000	-2.33239500	0.00000000
B	0.91711500	0.70548800	-1.69665200
B	-0.47592300	-1.72955900	-1.35377900
B	0.91711500	0.70548800	1.69665200
B	0.33344600	1.98597800	-0.80997600
B	-0.71347400	1.23762400	-1.78837200
B	-0.41616500	-0.28660400	-2.11843600
B	0.33344600	1.98597800	0.80997600
B	-0.47592300	-1.72955900	1.35377900
B	1.07303500	-0.83895400	-1.36710900
Fe	-0.32613600	0.01947100	0.00000000
Li	-1.64028400	2.46299000	0.00000000
Li	2.29597000	0.52298300	0.00000000



C_s-$^3A'$

E+ZPE= -1626.800270 au

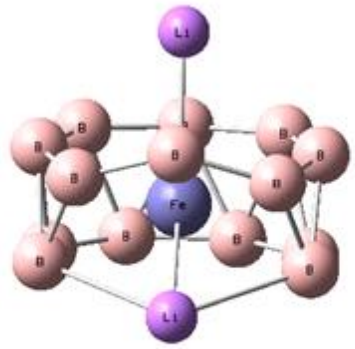
B	-0.69949100	0.75555300	1.83495200
B	-1.19304300	-0.98710800	1.46051800
B	-1.86007700	-1.04054600	0.00000000
B	0.88576300	0.90630300	1.77518200
B	2.15949700	-0.87631600	0.00000000
B	-0.69949100	0.75555300	-1.83495200
B	1.75922300	-0.44625600	-1.44987800
B	-1.89393000	0.53634700	0.79394900
B	1.75922300	-0.44625600	1.44987800
B	-1.19304300	-0.98710800	-1.46051800
B	0.25396500	-0.68674200	-2.08077000
B	-1.89393000	0.53634700	-0.79394900
B	0.25396500	-0.68674200	2.08077000
B	0.88576300	0.90630300	-1.77518200
Fe	0.08541000	-0.07985800	0.00000000
Li	2.34473000	1.34684500	0.00000000
Li	-0.62560700	2.27971200	0.00000000



C_s-^{1}A'

E+ZPE= -1626.798322 au

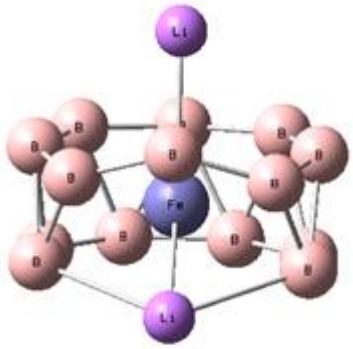
B	-0.68031400	0.81060300	1.85046900
B	-1.24891500	-0.89382100	1.47966600
B	-1.91808700	-0.94251600	0.00000000
B	0.90070100	0.92880200	1.76790900
B	2.18182400	-0.86367500	0.00000000
B	-0.68031400	0.81060300	-1.85046900
B	1.74191600	-0.42923300	-1.43111000
B	-1.85341500	0.61353500	0.78938400
B	1.74191600	-0.42923300	1.43111000
B	-1.24891500	-0.89382100	-1.47966600
B	0.22508500	-0.63478200	-2.06052700
B	-1.85341500	0.61353500	-0.78938400
B	0.22508500	-0.63478200	2.06052700
B	0.90070100	0.92880200	-1.76790900
Fe	0.07327100	-0.21133600	0.00000000
Li	2.35353400	1.34814300	0.00000000
Li	-0.37830600	2.17674000	0.00000000



C_s-^{1}A'

E+ZPE= -1626.795889 au

B	-0.00073800	2.14286800	0.82529300
B	-2.01711900	0.19423600	0.65922100
B	1.92857600	0.92456200	-0.90083800
B	1.87591800	-0.65581300	-0.89399300
B	-1.92877200	0.92317200	-0.90095300
B	0.00062200	-1.95060100	0.77313400
B	-1.87661200	-0.65721200	-0.89307300
B	1.44784500	1.74391900	0.41011400
B	1.44203600	-1.27947400	0.78602100
B	0.79636300	-1.84324800	-0.81019500
B	-0.79668400	-1.84409900	-0.80953700
B	2.01724900	0.19457900	0.65843000
B	-1.44920800	1.74369700	0.40995300
B	-1.44061100	-1.27918600	0.78747700
Fe	-0.00010500	0.08899200	-0.11424500
Li	0.00001500	2.23626600	-1.49137800
Li	0.00278300	-0.26986500	2.31307700



C_s-^{3}A'

T + ZPE = -1626.792447 au

B	-0.00073800	2.14286800	0.82529300
B	-2.01711900	0.19423600	0.65922100
B	1.92857600	0.92456200	-0.90083800
B	1.87591800	-0.65581300	-0.89399300
B	-1.92877200	0.92317200	-0.90095300
B	0.00062200	-1.95060100	0.77313400
B	-1.87661200	-0.65721200	-0.89307300
B	1.44784500	1.74391900	0.41011400
B	1.44203600	-1.27947400	0.78602100
B	0.79636300	-1.84324800	-0.81019500
B	-0.79668400	-1.84409900	-0.80953700
B	2.01724900	0.19457900	0.65843000
B	-1.44920800	1.74369700	0.40995300
B	-1.44061100	-1.27918600	0.78747700
Fe	-0.00010500	0.08899200	-0.11424500
Li	0.00001500	2.23626600	-1.49137800
Li	0.00278300	-0.26986500	2.31307700

Table S1: Cartesian Coordinates (angstrom) of some lower-lying isomers of Li_2FeB_{14}.