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

Supporting Information

Beryllium-Beryllium only double-π bonds in the octahedral cluster of $Be_2(\mu_2\text{-}X)_4$ (X=Li, Cu, BeF)

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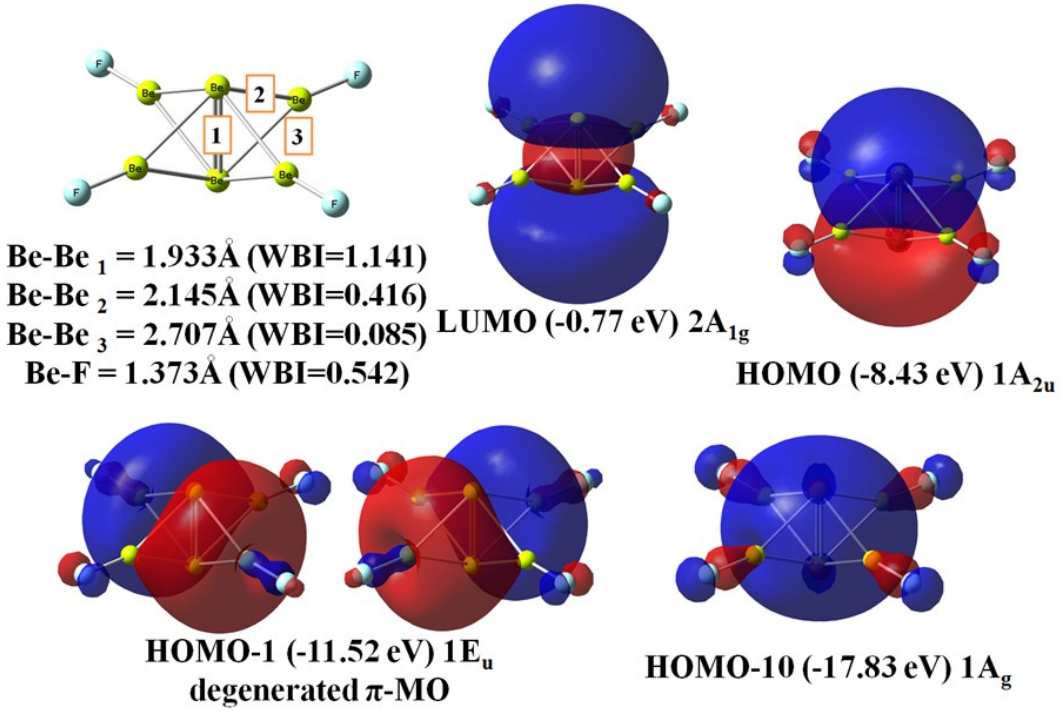


Figure S1. The global minimum of $Be_2(BeF)_4$ with the D_{4h} symmetry and its important FMOs under CCSD/cc-pVTZ level. It should be noted that the isolated orbitals of F from HOMO-9 to HOMO-2 have been omitted here.

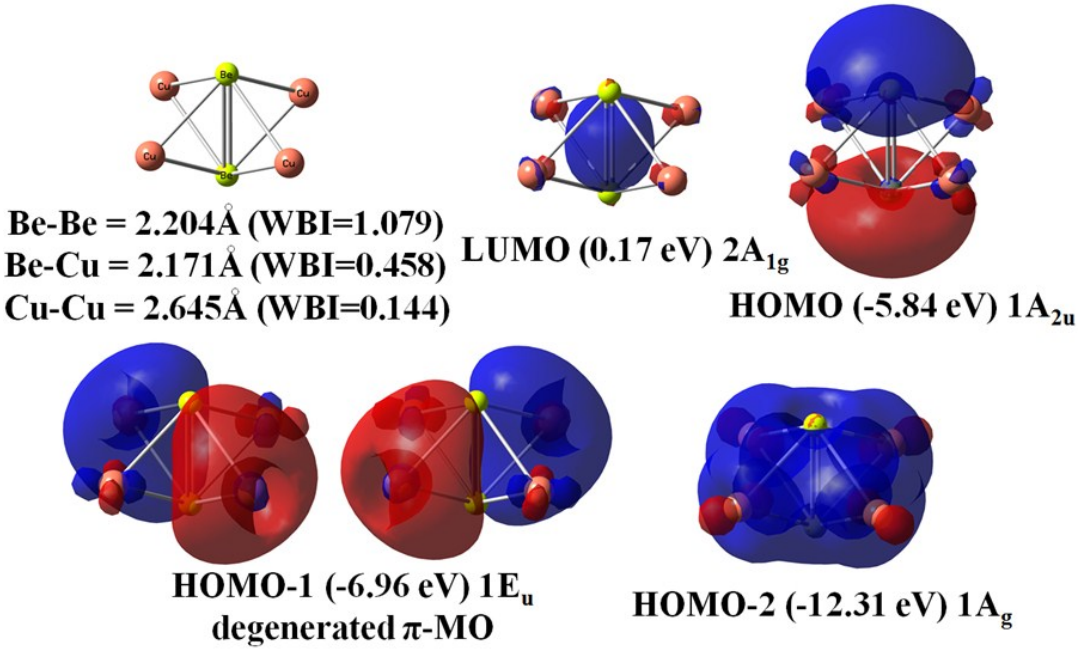


Figure S2. The global minimum of $Be_2(Cu)_4$ with the D_{4h} symmetry and its important FMOs under CCSD/cc-pVTZ/LANL2DZ level. The inner orbital of Cu and Be omitted here.

SI2

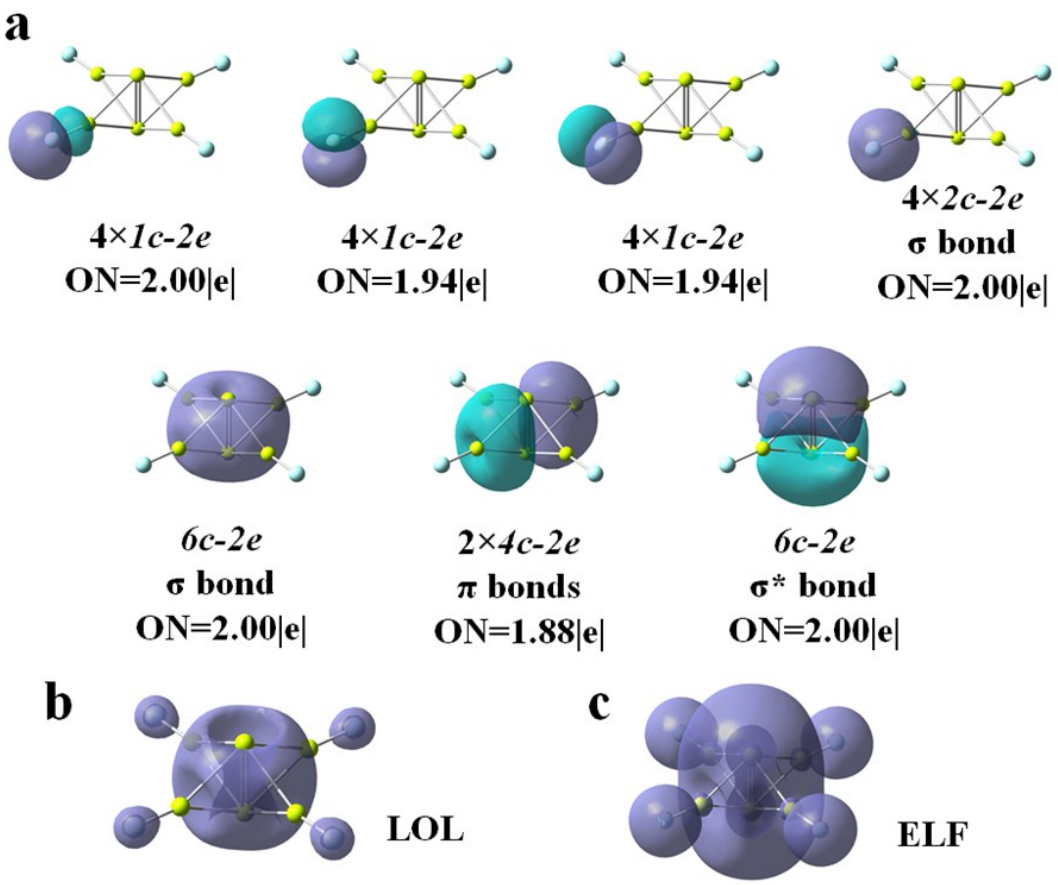


Figure S3. a) AdNDP orbitals. **b)** LOL profile. **c)** ELF profile for $Be_2(BeF)_4$ did under CCSD/cc-pVTZ level. ON stands for the occupation number.

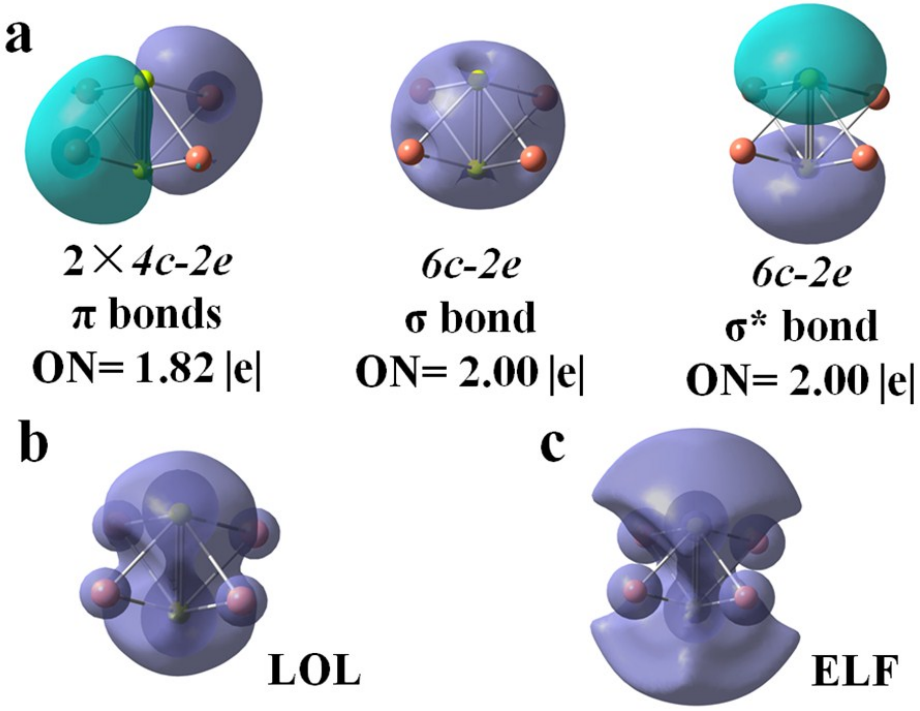


Figure S4. a) AdNDP orbitals. **b)** LOL profile. **c)** ELF profile for Be_2Cu_4 under CCSD/cc-pVTZ/LANL2DZ level. ON stands for the occupation number.

SI3

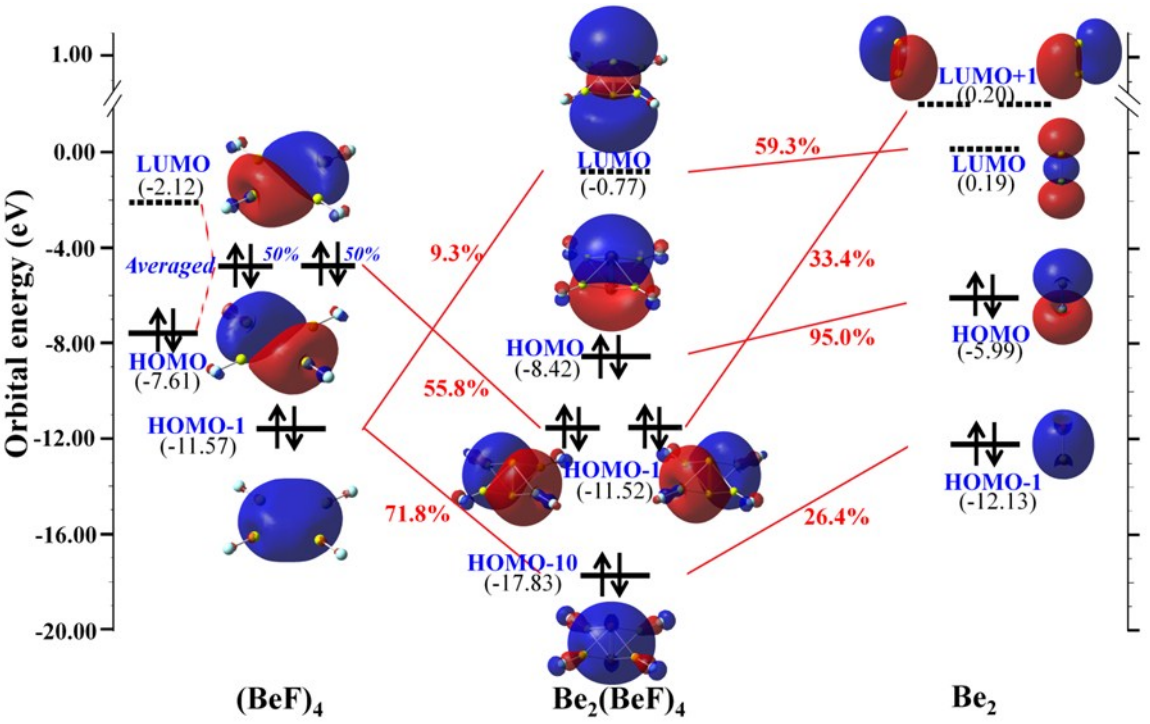


Figure S5. The dominant FMOs correlation diagram in $Be_2(BeF)_4$ under CCSD/cc-pVTZ level between vertex-Be_2 and $(BeF)_4$ fragments.

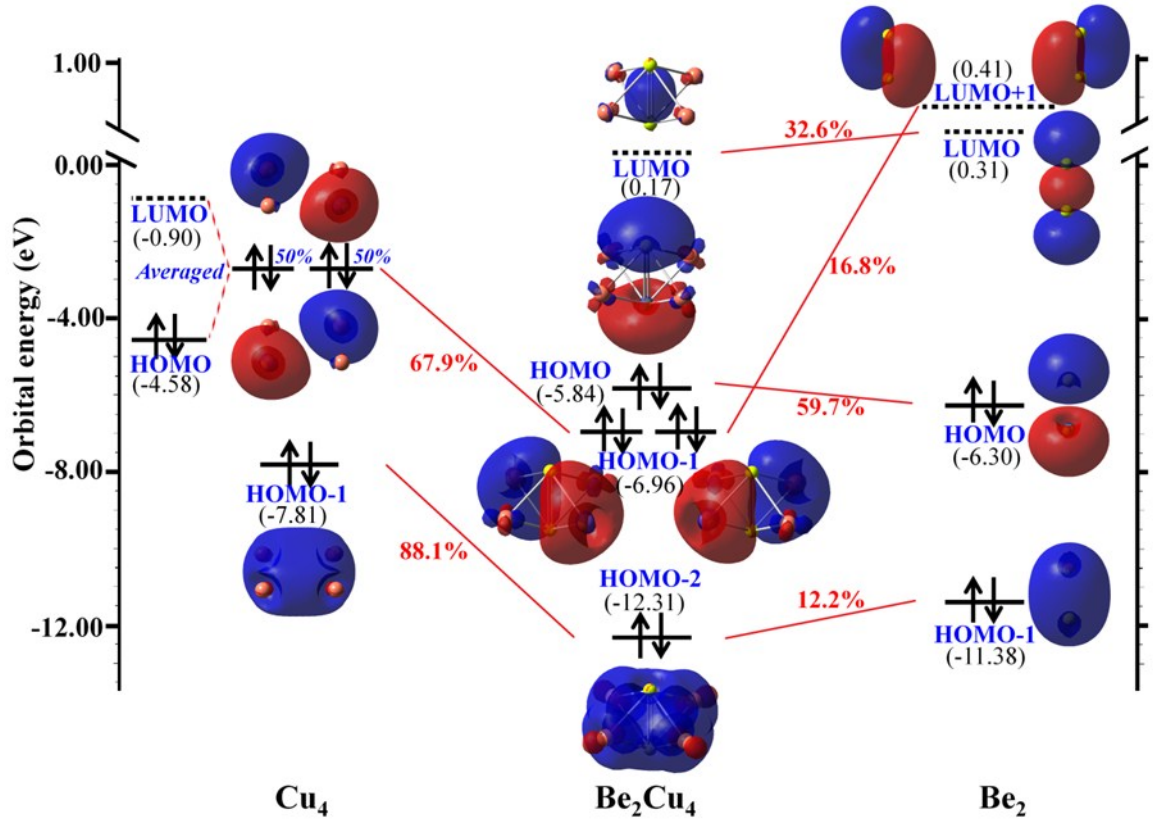


Figure S6. The dominant FMOs correlation diagram under CCSD/cc-pVTZ/LANL2DZ level in Be_2Cu_4 between Be_2 and Cu_4 fragments.

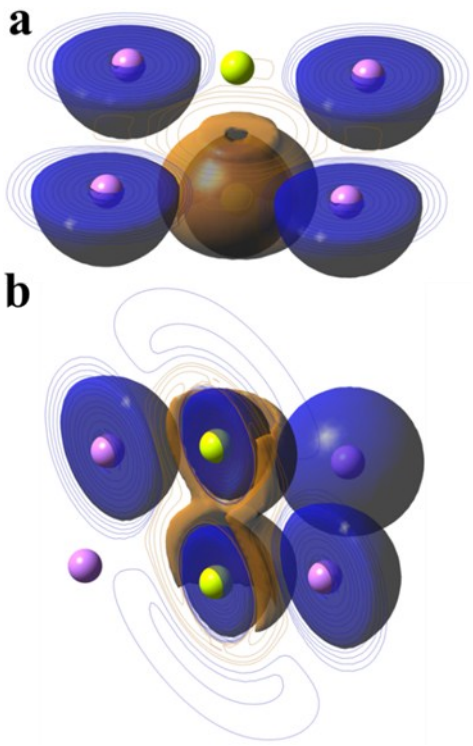


Figure S7. Laplacian plot of the electron density $\nabla^2\rho(r)$ of Be_2Li_4 under CCSD/cc-pVTZ level in different perspectives. **a)** The plane of the Li_4 ring from the vertical view. **b)** Front view that contains two vertex-Be atoms and two opposing Li atoms bisecting the plane of the Li_4 ring. The orange lines including corresponding region indicate the areas of charge concentration ($\nabla^2\rho(r)<0$) while blue lines and corresponding region show the areas of charge depletion ($\nabla^2\rho(r)>0$).

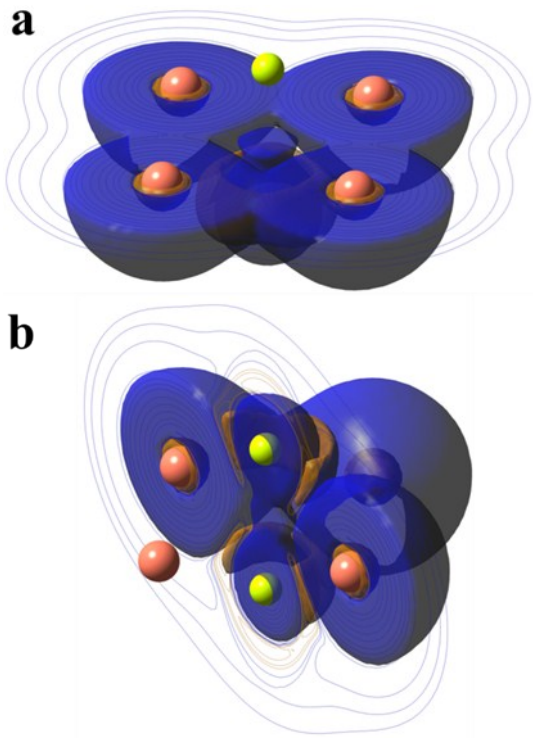


Figure S8. Laplacian plot of the electron density $\nabla^2\rho(r)$ of Be_2Cu_4 under CCSD/cc-pVTZ/LANL2DZ level in different perspectives. **a)** The plane of the Cu_4 ring from the vertical view. **b)** Front view that contains two vertex-Be atoms and two opposing Cu atoms bisecting the plane of the Cu_4 ring. The orange lines including corresponding region indicate the areas of charge concentration ($\nabla^2\rho(r)<0$) while blue lines and corresponding region show the areas of charge depletion ($\nabla^2\rho(r)>0$).

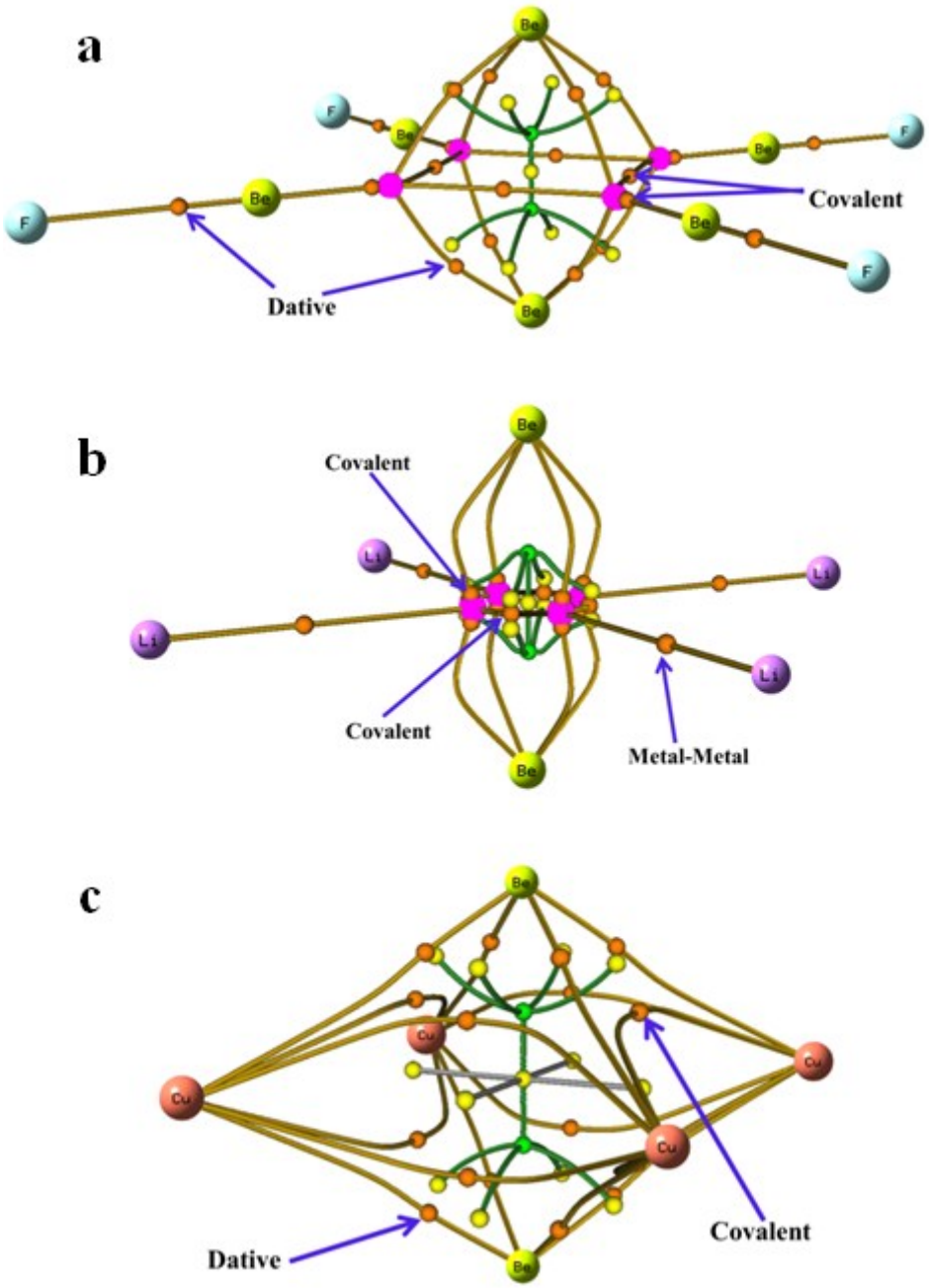


Figure S9. AIM results under the same level as their optimization progress for **a)** $Be_2(BeF)_4$, **b)** Be_2Li_4 and **c)** Be_2Cu_4. It is clear that there no BCP along Be-Be axle meaning there no direct σ bonding interaction between two Be atom. Here the orange dots are bond critical points(BCP), yellow dots are ring critical points(RCP), and the two green dots are the cage critical points(CCP). The purple dots in $Be_2(BeF)_4$ and Be_2Li_4 including two parts. In addition to the nucleus critical points(NCP), the "Non-nuclesr-attractor(**NNA**)" is marked pink color.(Please refer to *Organometallics* **2013**, 32, 1060−1066; *Inorg. Chem*. **2000**, 39, 2360-2366 and *Angew. Chem. Int. Ed.* **1984**, 23 627−628) There exist four **NNA**s in both in $Be_2(BeF)_4$ and Be_2Li_4 separately. The orange solid lines represent the path connected the BCP and NCP and the green solid lines connected RCP and CCP. Indicators in the graph: *Covalent* indicates the covalent bond, *Dative* indicates the dative bond, *Metal-Metal* means the metallic bond.

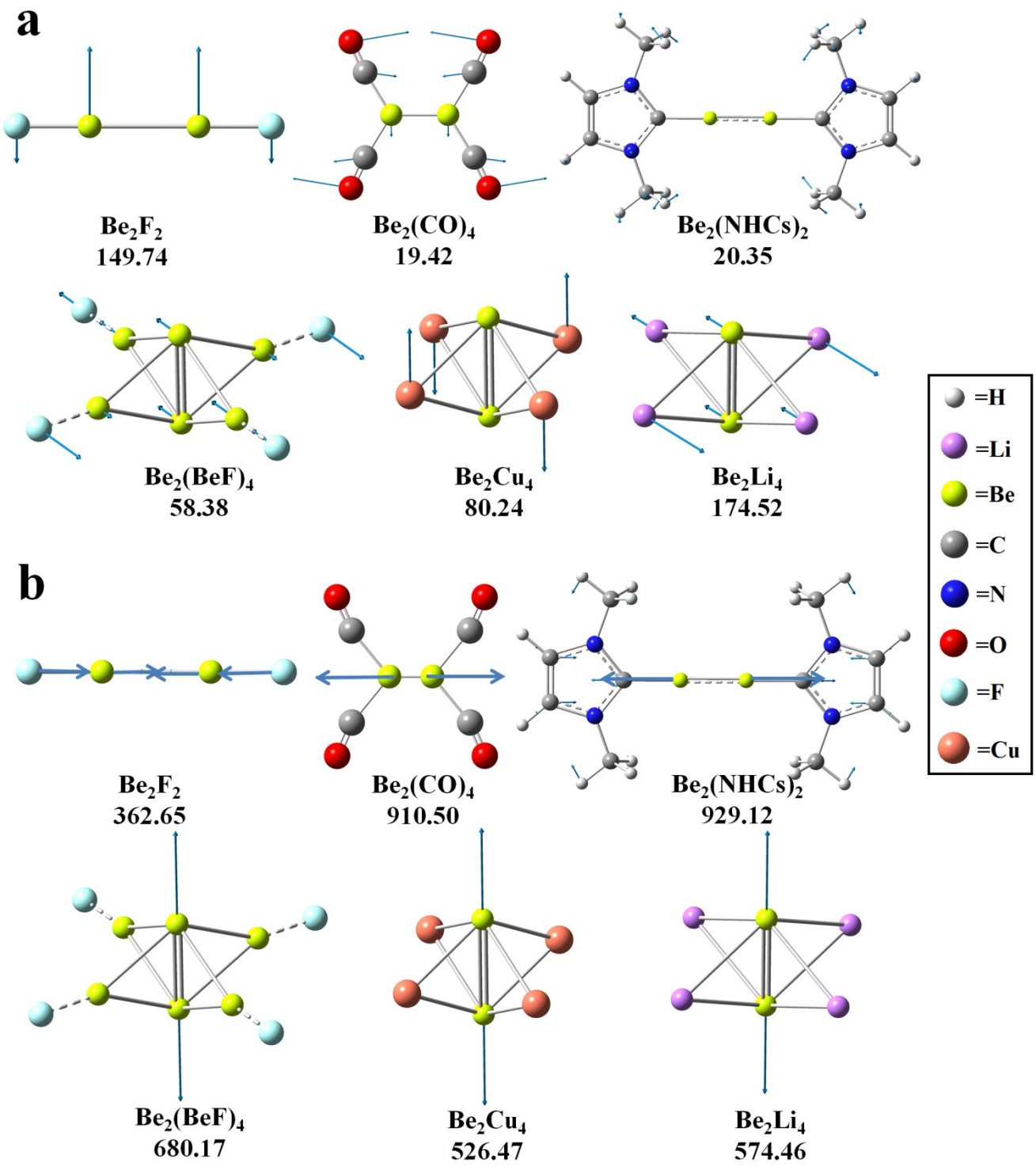
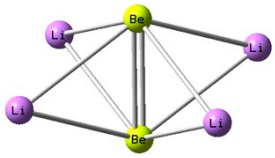
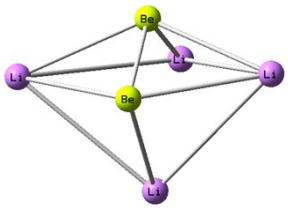


Figure S10. a) The lowest frequency and the corresponding vibrational modes. **b)** The normal modes of Be-Be stretching vibrational frequency in Be_2-containing complexes under the same level as their optimization progress. (unit: cm^{-1}.)

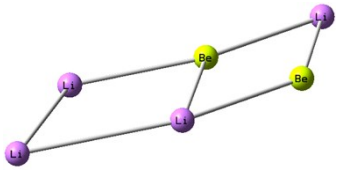
SI7



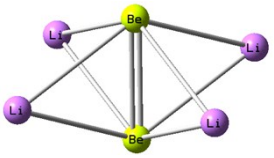
0.0
1a (D_{4h}, ^1A)



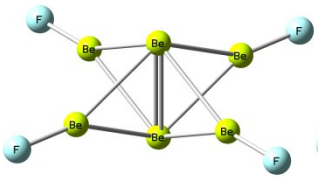
11.9
1b (C_s, ^1A)



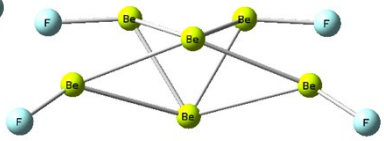
36.2
1c (C_s, ^1A)



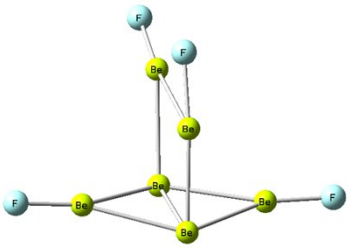
20.0
1d (D_{4h}, ^3A)



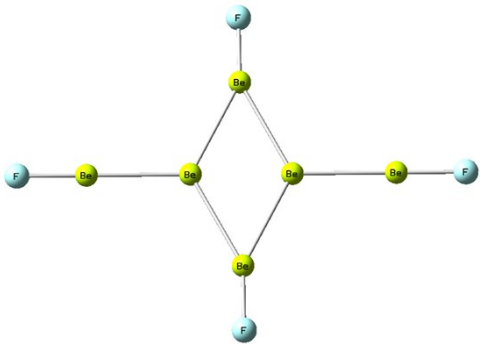
0.0
2a (D_{4h}, ^1A)



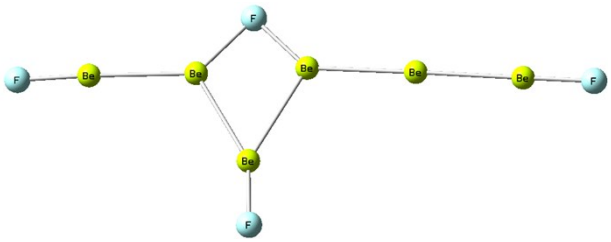
4.9
2b (C_{2v}, ^1A)



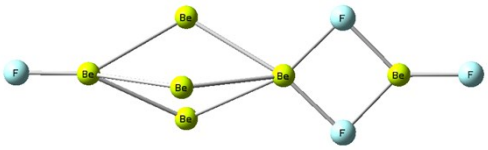
7.8
2c (C_s, ^1A)



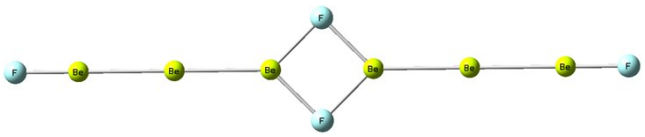
10.2
2d (C_{2h}, ^1A)



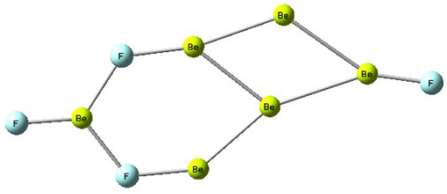
18.0
2e (C_{2h}, $^1A'$)



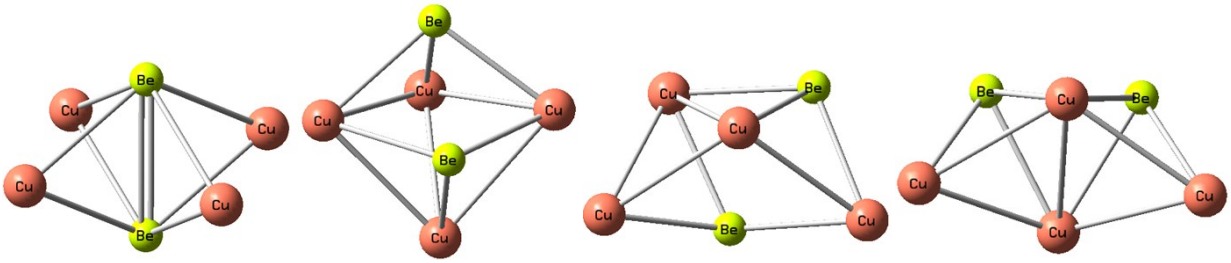
18.2
2f (C_s, ^1A)



19.6
2g (D_{2h}, ^1A)



26.7
2h (C_s, $^3A''$)

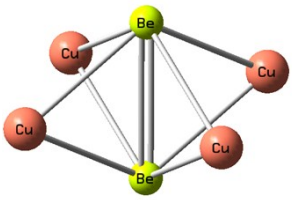


0.0 **3a** (D_{4h}, ^{1}A)

12.8 **3b** (C_{2v}, ^{1}A)

15.8 **3c** (C_1, ^{1}A)

24.0 **3d** (C_{2v}, ^{1}A)



35.4 **3e** (D_{4h}, ^{3}A)

Figure S11. The lowest-lying isomers of Be_2Li_4, $Be_2(BeF)_4$ and Be_2Cu_4 shortened as **1**, **2** and **3** respectively with energy in kcal/mol using G3B3 approach (please refer to *J. Chem. Phys.* 109, **1998**, 7764). **1d**, **2h** and **3e** represent the lowest triplet isomers on the PES, respectively. It is noteworthy that many of the structures will be transformed to the octahedral conformation after the re-optimization under higher basis set level, so some transformed isomers are omitted here.

SI8

Table S1. The orbital composition of Be_2Li_4 under CCSD/cc-pVTZ level. The molecular orbitals originated from the inner shell AOs are omitted. The coefficient of each orbital is given by the contribution from the Be_2 and Li_4 fragments. The same way for Be_2Cu_4 $Be_2(BeF)_4$.

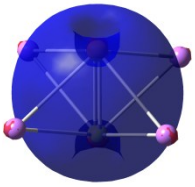
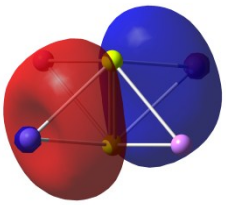
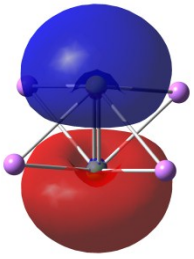
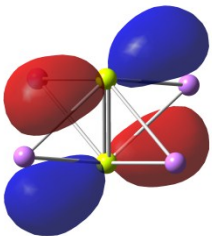
Be_2Li_4	Occupied molecular orbital			Unoccupied molecular orbital
	σ	2×π	σ*	2×π*
Diagram				
Energy/eV	-11.15	-5.19	-5.03	2.98
Component	Li_4©2s~30.4% Be_2©2s~53.0%	Li_4©2s~65.3% Be_2©$2p_{x,y}$~18.7%	Be_2©2s~94.4%	Li_4©$2p_z$~38.4% Be_2©$2p_{x,y}$~59.7%

Table S2. The orbital composition of **Be_2Cu_4** under CCSD/cc-pVTZ/LANL2DZ level

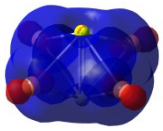
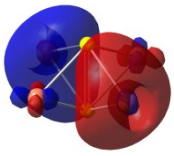
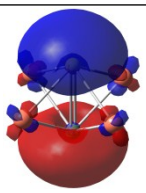
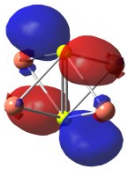
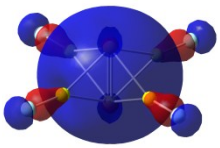
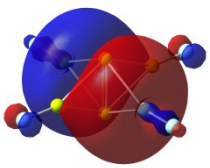
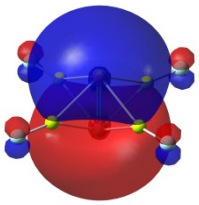
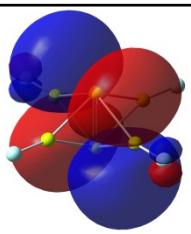
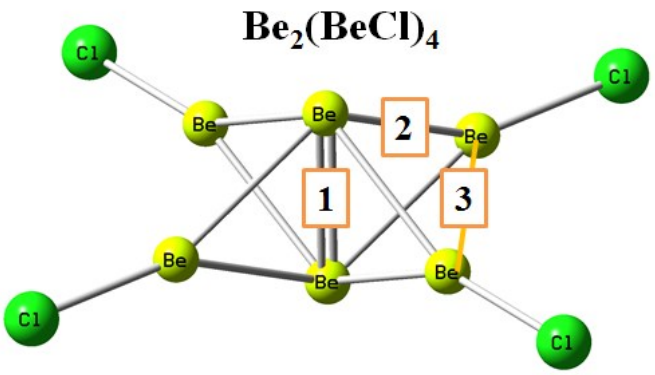
Be_2Cu_4	Occupied molecular orbital			Unoccupied molecular orbital
	σ	2×π	σ*	2×π*
Diagram				
Energy/eV	-12.31	-6.96	-5.84	2.98
Component	Cu_4©4s~21.8% Cu_4©$3dz^2$~35.6% Be_2©2s~33.4%	Cu_4©4s~63.5% Cu_4©$4p_{x,y}$~9.2% Cu_4©dx^2-y^2~7.8% Cu_4©3s~7.1% Be_2©$2p_{x,y}$~10.5%	Cu_4©$4p_z$~10.7% Cu_4©d_{xy}~5.0% Cu_4©d_{yz}~5.0% Be_2©2s~53.2% Be_2©$2p_z$~19.9%	Cu_4©$4p_z$~46.4% Be_2©$2p_{x,y}$~52.7%

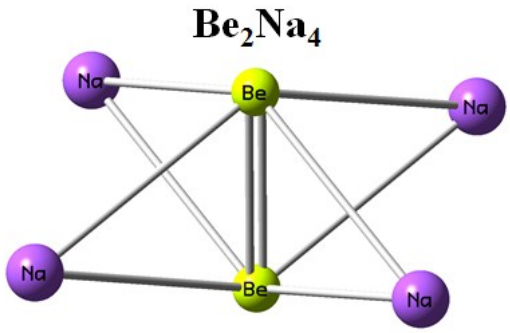
Table S3. The orbital composition of **$Be_2(BeF)_4$** under CCSD/cc-pVTZ level.

$Be_2(BeF)_4$	occupied molecular orbital			unoccupied molecular orbital
	σ	2×π	σ*	2×π*
Diagram				
Energy/eV	-17.39	-11.52	-8.43	-0.18
Component	Be_4©2s~16.6% Be_4©$2p_{x,y}$~7.5% Be_4©2pz~5.6% F_4©$2p_{x,y}$~6.8% Be_2©2s~56.7%	Be_4©2s~42.1% Be_4©$2p_{x,y}$~19.7% Be_2©$2p_{x,y}$~24.9%	Be_2©2s~92.3%	Be_4©$2p_z$~8.8% Be_2©$2p_{x,y}$~88.2%



Be-Be-1 = 1.891Å (WBI=1.113)
Be-Be-2 = 2.108Å (WBI=0.477)
Be-Be-3 = 2.663Å (WBI=0.136)
Be-Cl = 1.807Å (WBI=1.039)

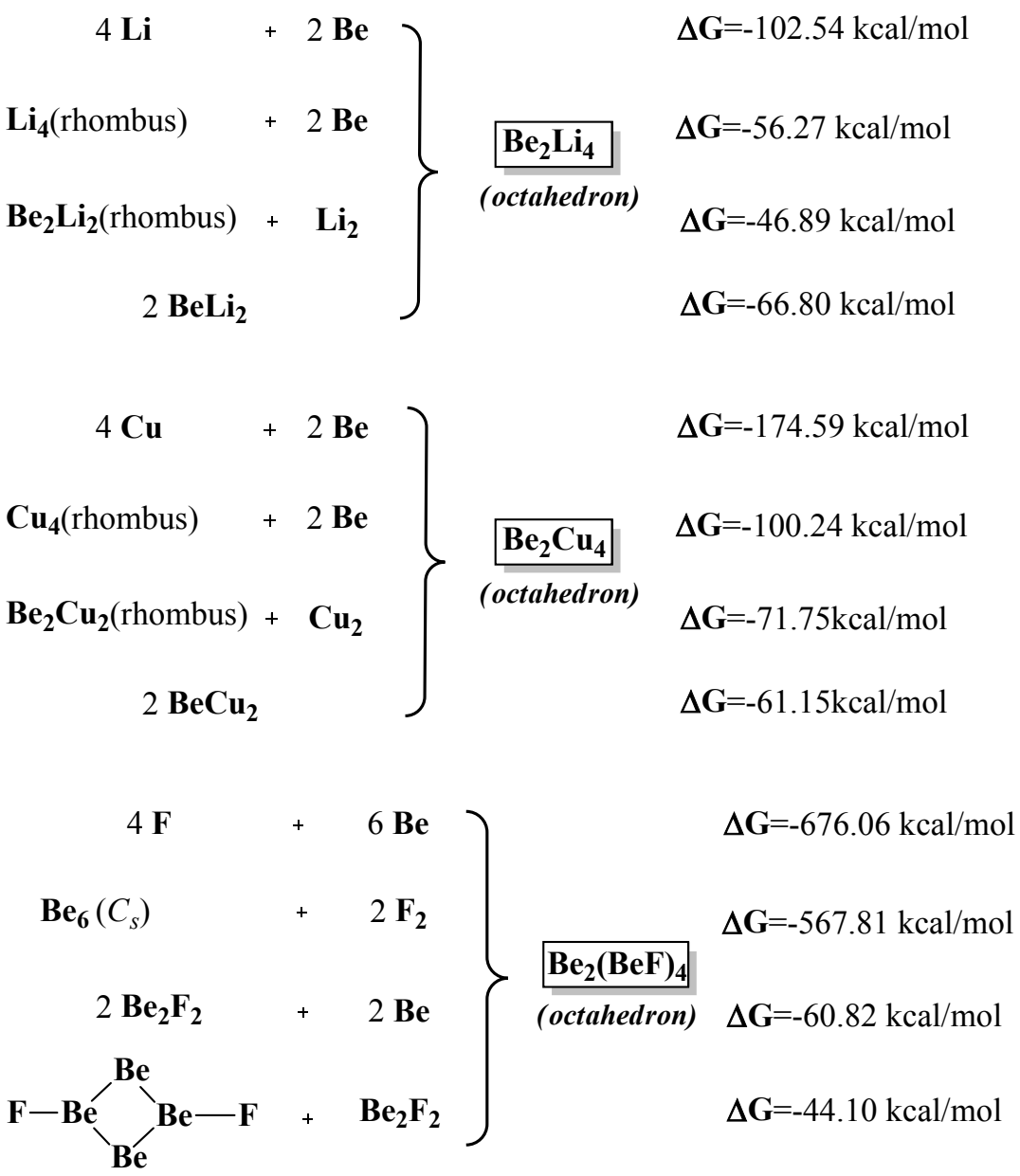
NPA(vertex-Be) = -0.27
Lowest frequency= 32.63 cm^{-1}
Be-Be stretching vibration frequency= 698.15 cm^{-1}



Be-Be = 2.115Å (WBI=2.376)
Be-Na = 2.774Å (WBI=0.302)
Na-Na = 3.630Å (WBI=0.031)

NPA(vertex-Be) = -1.26
Lowest frequency= 59.58 cm^{-1}
Be-Be stretching vibration frequency= 503.97 cm^{-1}

Figure S12. The data on other two optimized structures by this universal strategy including $Be_2(BeCl)_4$ and Be_2Na_4 under B3LYP/cc-pVTZ level. The same conclusion can be drawn, since the same trend is for $Be_2(BeF)_4$, Be_2Cu_4, Be_2Li_4 under the same level. The frequency analysis is achieved also under B3LYP/cc-pVTZ level. They are all the lowest-energy structure under this level. The most-important bond-lengths and WBIs for $Be_2(BeCl)_4$ and Be_2Na_4 are also shown under CCSD/cc-pVTZ level.



Scheme S1. Several possible reactions and thermodynamic values for the generation of octahedral Be_2Li_4, Be_2Cu_4 and $Be_2(BeF)_4$ using CCSD method. The LANL2DZ basis set for Cu, cc-pVTZ for Be, Li and F. The Gibbs free energy differences (ΔG) of all reactions are always negative, so in thermodynamics, Be_2Cu_4, Be_2Li_4 and $Be_2(BeF)_4$ are stable and can most likely be obtained by some reactions.

SI11

The octahedral Be_2X_4 (X = Li, Cu, BeF) structures is optimized and calculated at the CASSCF(8,8)/6-31G* level. These active orbitals are including 4 σ and 4 π orbitals, in which 6 orbitals (2 σ + 4 π) are shown in SI8. Since the 2 σ orbitals in SI8 are occupied, we introduced LUMO (σ orbital) and the corresponding σ* orbital in the active space.
As expected, the CASSCF(8,8) results are consistent with the CCSD results. All the dominant configurations in octahedral Be_2X_4 (X = Li, Cu, BeF) are the degenerate double-π bonds state, and the corresponding weights are all over 83%. It is suggested that there are no multi-reference configurations in nature.

Table S4. The weight of degenerate double-π bonds configuration under CASSCF(8,8)/6-31G* level for the global minimums.

	Be_2Li_4	**Be_2Cu_4**	**$Be_2(BeF)_4$**
Basis set	6-31G*	6-31G*/LANL2DZ	6-31G*
Weight (%)	83.08	86.27	86.17

SI12

Coordinates and energies (unit: a.u.) of Be_2Li_4, $Be_2(BeF)_4$, Be_2Cu_4, $Be_2(BeCl)_4$, Be_2Na_4, Be_2, Be_2F_2, $Be_2(CO)_4$, $Be_2(NHCs)_2$.
Methods and Basis Sets are shown in brackets.

Part-A
Be_2Li_4 (octahedron)
(CCSD/cc-pVTZ)
E= -58.9898646

Li	0.00000000	-2.23938318	0.00000000
Li	0.00000000	2.23938318	0.00000000
Li	2.23938318	0.00000000	0.00000000
Li	-2.23938318	0.00000000	0.00000000
Be	0.00000000	0.00000000	-1.02046995
Be	0.00000000	0.00000000	1.02046995

Be_2Cu_4(octahedron)
(CCSD/LANL2DZ/cc-pVTZ)
E= -809.2443965

Cu	0.00000000	1.87019576	0.00000000
Cu	0.00000000	-1.87019576	0.00000000
Cu	-1.87019576	0.00000000	0.00000000
Cu	1.87019576	0.00000000	0.00000000
Be	0.00000000	0.00000000	-1.10201255
Be	0.00000000	0.00000000	1.10201255

$Be_2(BeF)_4$(octahedron)
(CCSD/cc-pVTZ)
E= -486.0388955

Be	0.00000000	0.00000000	-0.96641617
Be	0.00000000	0.00000000	0.96641617
Be	-1.91449602	0.00000000	0.00000000
Be	0.00000000	-1.91449602	0.00000000
Be	0.00000000	1.91449602	0.00000000
Be	1.91449602	0.00000000	0.00000000
F	3.28754771	0.00000000	0.00000000
F	0.00000000	-3.28754771	0.00000000
F	0.00000000	3.28754771	0.00000000
F	-3.28754771	0.00000000	0.00000000

Be_2Na_4(octahedron, shown as Figure S12)
(B3LYP/cc-pVTZ)

E=-678.6918297

Be	-0.00100181	-0.00042887	-1.06244913
Be	0.00040200	-0.0012882	1.05280627
Na	1.81649517	-1.81503023	-0.00054721
Na	1.81489523	1.81529882	0.00099420
Na	-1.81472134	1.81593194	-0.00069130
Na	-1.81688527	-1.81524841	0.00178317

$Be_2(BeCl)_4$(octahedron, shown as Figure S12)
(B3LYP/cc-pVTZ)
E=-1929.7278250

Be	1.33140015	1.33106980	-0.00213893
Be	-1.33130294	1.33179229	-0.00217000
Be	1.33168108	-1.33138681	-0.0022735
Be	-0.00037739	-0.00032762	-0.94543804
Be	-1.33200648	-1.33168635	-0.00173043
Be	-0.00019332	-0.00021839	0.94519316
Cl	2.60932212	2.60850134	-0.00045929
Cl	2.60942136	-2.60898419	0.00040036
Cl	-2.60990641	-2.60911149	-0.00037425
Cl	-2.60872216	2.60971043	0.00042100

Part-B
The lowest-lying isomers coordinates of Be_2Li_4, $Be_2(BeF)_4$ and Be_2Cu_4 respectively using G3B3 approach.

Be_2Li_4
(B3LYP/6-31g*)

1a
E=-59.5301406

Li	1.61488693	1.51975824	-0.00310694
Li	-1.5155076	1.6183457	-0.00295309
Li	-1.61800449	-1.51795305	-0.00488208
Be	-0.00022415	0.00052327	1.01301859
Be	-0.00021821	0.00058569	-1.00493650
Li	1.51826361	-1.61835386	-0.00235397

1b
E=-59.5111688

Li	0.00367008	2.3133411	0.02915767
Li	-2.21087718	-0.27958940	-0.19743660
Be	0.00026486	0.18523871	-1.08406589
Li	-0.00005348	0.00842115	1.85489343
Be	-0.0022962	-1.49944636	-0.03193017
Li	2.20998898	-0.28631827	-0.19740344

1c
E=-59.4724326

Li	-1.66171083	3.03301595	0.00000000
Li	2.17053963	-0.30441158	0.00000000
Be	0.00325070	1.11301659	0.00000000
Li	2.37231020	-3.25027558	0.00000000
Li	-0.25921979	-1.53923148	0.00000000
Be	-1.96844391	0.43595310	0.00000000

1d
E=-59.4982230

Li	-1.61272600	1.57777300	0.02809300
Li	-1.58902900	-1.60175400	-0.02921800
Be	-0.00040400	0.07374500	-0.93869300
Li	1.61347500	-1.57766800	-0.03020800
Li	1.58804500	1.60254100	0.02921000
Be	0.00057900	-0.07441400	0.94028500

$Be_2(BeF)_4$
(B3LYP/6-31g*)

2a
E=-488.1742492

Be	1.33028100	1.33156300	-0.00095800
Be	-1.33174400	1.33061200	-0.00125300
Be	1.33222200	-1.33009700	-0.00168400
Be	-0.00026300	-0.00010200	-0.96070200
Be	-1.33075800	-1.33207200	-0.0011700
Be	-0.00019100	-0.00034500	0.96325100
F	-2.30671200	-2.30892400	-0.00066600
F	-2.30861900	2.30655700	0.00088600
F	2.30927800	-2.3058600	0.00035200
F	2.30625500	2.30842200	0.00054700

2b
E=-488.1616517

Be	2.15101100	0.45774200	-0.00002900
Be	-1.04308800	-1.28823300	-0.00213600
Be	1.04318200	-1.28858200	0.00134700
Be	-2.15131600	0.45744300	0.00034400
Be	0.00065500	0.25993900	-0.96142300
Be	-0.00061200	0.25900400	0.96236500
F	-2.53387400	-1.17706700	-0.00097700
F	3.14982100	1.43089400	-0.00097900
F	-3.14970000	1.43102900	0.00079900
F	2.53382800	-1.17699400	0.00095000

2c
E=-488.1618696

Be	-0.02364800	1.49391200	-0.24348000
Be	-1.86848000	-1.25037600	-0.25900500
Be	0.00972700	-0.15495200	1.10260000
Be	1.90339800	-1.21000700	-0.26330100
Be	0.02616600	-2.00585500	0.302185000
Be	0.01066300	-0.63362100	-0.98382700
F	3.283630000	-1.15783900	-0.19419800
F	-0.04410100	2.74262200	-0.85171500
F	-3.24938600	-1.22225000	-0.19192200
F	-0.01584400	1.30897700	1.39109100

2d
E=-488.1580211

Be	-3.06008800	-0.0074700	-0.00074600
Be	3.05968500	0.00867700	-0.00068800
Be	-1.00669300	-0.00499200	-0.00064700
Be	0.00979900	-1.95617300	-0.00066300
Be	1.00617500	0.00487600	0.00098200
Be	-0.0101800	1.95658200	0.00101200
F	-0.01445300	3.32998100	0.00204200
F	-4.43476500	-0.01073900	-0.00200400
F	0.01542900	-3.32957900	0.00248100
F	4.43436800	0.00966900	-0.00218700

2e
E=-488.1456297

Be	-3.4930200	-1.61653700	0.00000000
Be	-1.75759100	-0.50804200	0.00000000
Be	3.67483100	2.68641100	0.00000000
Be	0.20866400	-1.50523700	0.00000000
Be	1.83680700	1.71025800	0.00000000
Be	0.00000000	0.69725600	0.00000000
F	1.03063900	-2.61034500	0.00000000
F	-4.6165200	-2.41012500	0.00000000

F	-1.50617200	1.02710700	0.00000000
F	4.88330100	3.34264800	0.00000000

2f

E=-488.1452879

Be	2.58630800	0.00111100	-0.01375100
Be	-1.51090100	-0.97233500	-0.57450800
Be	0.37017800	-0.00567900	0.08727400
Be	-3.37972300	-0.00294700	-0.01181100
Be	-1.51095200	1.01911600	-0.49633800
Be	-1.5627800	-0.04608500	1.17197900
F	1.50846600	1.11753200	0.04143500
F	1.51377500	-1.12100100	0.04016600
F	-4.76783700	0.00228500	-0.06485900
F	3.97131500	0.00421500	-0.08911700

2g

E=-488.1430693

Be	3.2134700	-0.00030700	0.00007200
Be	1.11895900	-0.00059500	0.00002600
Be	5.29874400	-0.00001100	-0.00002800
Be	-3.21346400	0.00026500	-0.00004200
Be	-5.29873900	0.00017700	-0.0000600
Be	-1.1189500	0.00037500	-0.00011100
F	-6.67495100	0.00004700	0.00011700
F	0.00020400	1.11021900	-0.00006300
F	6.67495700	0.00023800	0.00007100
F	-0.00021900	-1.11046200	-0.00006300

2h

E=-488.1316917

Be	1.95240069	1.63874948	0.00000000
Be	-0.00030162	1.15042956	0.00000000
Be	-2.46631929	-0.13160316	0.00000000
Be	1.51588644	-0.26010853	0.00000000
Be	3.62381065	0.23398269	0.00000000
Be	-0.09142952	-1.43503588	0.00000000
F	-1.59941195	-1.4389777	0.00000000
F	-1.52969264	1.10034487	0.00000000
F	4.96567548	-0.08534722	0.00000000
F	-3.85170122	-0.10811010	0.00000000

Be_2Cu_4(B3LYP/6-31g*)

3a

E=-6590.6748090

Be	-0.00050500	-0.00063200	1.20944900
Cu	-1.07266600	1.23486900	-0.00803100
Cu	1.23529400	1.07244400	0.00806300
Cu	-1.23501600	-1.07228100	0.00802300
Be	-0.00036900	-0.00016000	-1.20942200
Cu	1.07250900	-1.23492300	-0.00805900

3b

E=-6590.6543950

Be	0.00090200	1.07938000	1.23141400
Cu	-0.00257700	1.14669600	-0.73632600
Cu	1.56310300	0.00000900	0.56664600
Cu	-1.56074900	-0.00185900	0.56911500
Cu	-0.00017600	-1.14444800	-0.73886000
Be	0.00199200	-1.08226600	1.22941500

3c

E=-6590.6496110

Be	0.14897600	0.02671800	-1.12755600
Be	0.90731300	1.37471600	0.42116000
Cu	-1.01705800	1.27359300	-0.06110900
Cu	2.00257700	-0.06417300	-0.45558300
Cu	0.24832300	-0.42010100	1.02457200
Cu	-1.37953600	-0.98262100	-0.41044600

3d

E=-6590.6366280

Cu	-1.86843000	-0.00035900	-0.32367400
Be	-1.01256400	0.00026100	1.45508300
Cu	0.00004400	-1.20275100	0.12317600
Be	1.01259000	0.00062000	1.45503800
Cu	1.86840600	-0.00034300	-0.32367900
Cu	-0.00002300	1.20333200	0.12278100

3e

E=-6590.618374

Be	-0.00025753	-0.00006760	1.08781047
Cu	-1.11000865	1.27798307	0.00011636
Cu	1.27801074	1.10981614	0.00010601
Cu	-1.27828804	-1.11004445	-0.00012099
Be	0.00003745	-0.00013474	-1.08796018
Cu	1.10975303	-1.27823541	0.00007132

Part-C (Other related molecular structural coordinates)

Be_2

(CCSD(T)/cc-pVTZ)

E=-29.2386696

Be	0.00000000	0.00000000	0.00000000
Be	0.00000000	0.00000000	2.53550897

Be_2F_2

(CCSD/cc-pVTZ)

E=-228.3959601

Be	-0.7123828347	1.53416147	0.00000000
Be	1.3371034147	1.53416147	0.00000000
F	2.7079248986	1.53416147	0.00000000
F	-2.0832043186	1.53416147	0.00000000

$Be_2(CO)_4$

(CCSD/cc-pVTZ)

E=-480.2805796

Be	-0.00000265	-0.96126575	0.00000000
Be	-0.00000317	0.96126575	0.00000000
C	1.44329392	-1.83424482	0.00000000
C	-1.44329504	-1.83425206	0.00000000
C	1.44329295	1.83424556	0.00000000
C	-1.44329601	1.83425132	0.00000000
O	2.47549134	-2.30583733	0.00000000
O	-2.47549001	-2.30584979	0.00000000
O	-2.47549084	2.30584936	0.00000000
O	2.47549052	2.30583776	0.00000000

$Be_2(NHCs)_2$

(B3LYP/cc-pVTZ)

E=-639.0586516

Be	0.97118156	-0.00004657	-0.00003107
Be	-0.97118177	0.000043778	-0.00003162
C	2.65762158	-0.00002236	0.00003710
N	3.50872301	1.08358220	0.00035158
N	3.50875062	-1.08360475	-0.00034306

C	4.82864131	0.675998294	0.00044329
C	4.82865836	-0.67598645	-0.00030322
C	-2.65762179	0.000021478	0.00003373
N	-3.50872455	-1.08358199	0.00035020
N	-3.50874944	1.08360492	-0.00034433
C	-4.82864233	-0.67599643	0.00043919
C	-4.82865766	0.67598831	-0.00030903
C	-3.03652342	2.44739201	-0.00073999
H	-2.42559021	2.63730918	0.885815274
H	-2.42481309	2.63644448	-0.88694101
H	-3.88486285	3.12770779	-0.00145285
C	-3.03646705	-2.44735817	0.00061464
H	-2.42557217	-2.63719958	-0.88598388
H	-2.42471035	-2.63645904	0.88677288
H	-3.88479048	-3.12769378	0.00131896
C	3.03652630	-2.44739244	-0.00074251
H	2.42559204	-2.63731201	0.88581152
H	2.42481750	-2.63644402	-0.88694479
H	3.88486660	-3.12770716	-0.00145545
C	3.03646377	2.44735778	0.00061299
H	2.42556837	2.63719646	-0.88598578
H	2.42470710	2.63645983	0.88677100
H	3.88478634	3.12769448	0.00131546
H	5.64631662	1.37297322	0.00079850
H	5.64635143	-1.37294051	-0.00063101
H	-5.64634985	1.37294338	-0.00063818
H	-5.64631851	-1.37297032	0.000794481