Supporting Information

The Nature of Lithium Bonding in $C_2H_2Li_2$, C_6Li_6, and Lithium Halide Dimers

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Table S1. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **10**.

Atom	Number	Natural Charge
C	1	-0.84
C	2	-0.88
C	3	-0.85
C	4	-0.88
C	5	-0.89
C	6	-0.83
Li	7	0.77
Li	8	0.89
Li	9	0.90
Li	10	0.87
Li	11	0.85
Li	12	0.89

Table S2. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **15**.

Atom	Number	Natural Charge
Li	1	0.74
C	2	-0.75
C	3	-0.98
C	4	-0.98
C	5	-0.75
C	6	-0.87
C	7	-0.87
Li	8	0.89
Li	9	0.89
Li	10	0.89
Li	11	0.90
Li	12	0.90

Table S3. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **9**.

Atom	Number	Natural Charge
C	1	-0.86
C	2	-0.86
C	3	-0.86
Li	4	0.86
Li	5	0.86
Li	6	0.86
C	7	-0.86
C	8	-0.86
C	9	-0.86
Li	10	0.86
Li	11	0.86
Li	12	0.86

Table S4. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **14**.

Atom	Number	Natural Charge
Li	1	0.81
C	2	-0.91
C	3	-0.82
C	4	-0.91
C	5	-0.82
C	6	-0.79
C	7	-0.91
Li	8	0.85
Li	9	0.88
Li	10	0.88
Li	11	0.83
Li	12	0.90

Table S5. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **13**.

Atom	Number	Natural Charge
Li	1	0.92
C	2	-0.88
C	3	-0.88
C	4	-0.85
C	5	-0.85
C	6	-0.85
C	7	-0.85
Li	8	0.86
Li	9	0.86
Li	10	0.86
Li	11	0.83
Li	12	0.83

Table S6. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **12**.

Atom	Number	Natural Charge
Li	1	0.92
C	2	-0.86
C	3	-0.86
C	4	-0.85
C	5	-0.85
C	6	-0.85
C	7	-0.85
Li	8	0.83
Li	9	0.85
Li	10	0.83
Li	11	0.84
Li	12	0.84

Table S7. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **11**.

Atom	Number	Natural Charge
Li	1	0.62
C	2	-0.84
C	3	-0.84
C	4	-0.84
C	5	-0.84
C	6	-0.84
C	7	-0.84
Li	8	0.87
Li	9	0.87
Li	10	0.87
Li	11	0.91
Li	12	0.91

Table S8. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **8**.

Atom	Number	Natural Charge
C	1	-0.73
C	2	-0.83
C	3	-0.83
C	4	-0.73
C	5	-0.83
C	6	-0.83
Li	7	0.80
Li	8	0.79
Li	9	0.79
Li	10	0.80
Li	11	0.79
Li	12	0.79

Table S9. Result of natural charge at the ωB97XD/cc-pVQZ level for the structure **7**.

Atom	Number	Natural Charge
C	1	-0.64
C	2	-0.61
C	3	-0.61
C	4	-0.64
C	5	-0.61
C	6	-0.61
Li	7	0.62
Li	8	0.62
Li	9	0.62
Li	10	0.62
Li	11	0.62
Li	12	0.62

Table S10. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **10**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.00											
2	C	2.98	0.00										
3	C	0.01	0.01	0.00									
4	C	0.01	0.01	0.02	0.00								
5	C	0.01	0.02	2.98	0.01	0.00							
6	C	0.02	0.01	0.01	2.99	0.01	0.00						
7	Li	0.07	0.07	0.05	0.07	0.03	0.08	0.00					
8	Li	0.10	0.01	0.00	0.01	0.00	0.10	0.01	0.00				
9	Li	0.00	0.00	0.08	0.09	0.01	0.01	0.01	0.00	0.00			
10	Li	0.07	0.06	0.01	0.00	0.09	0.00	0.01	0.00	0.00	0.00		
11	Li	0.00	0.00	0.04	0.07	0.07	0.07	0.02	0.00	0.01	0.00	0.00	
12	Li	0.01	0.10	0.05	0.00	0.05	0.00	0.01	0.00	0.00	0.01	0.00	0.00

Table S11. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **15**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.00											
2	C	0.10	0.00										
3	C	0.06	2.97	0.00									
4	C	0.06	0.01	0.01	0.00								
5	C	0.10	0.02	0.01	2.97	0.00							
6	C	0.06	0.01	0.02	0.02	0.01	0.00						
7	C	0.06	0.01	0.02	0.02	0.01	2.96	0.00					
8	Li	0.01	0.10	0.01	0.01	0.10	0.00	0.00	0.00				
9	Li	0.01	0.00	0.00	0.10	0.01	0.04	0.05	0.00	0.00			
10	Li	0.01	0.01	0.10	0.00	0.00	0.05	0.04	0.00	0.00	0.00		
11	Li	0.01	0.00	0.00	0.08	0.03	0.08	0.01	0.00	0.01	0.00	0.00	
12	Li	0.01	0.03	0.08	0.00	0.00	0.01	0.08	0.00	0.00	0.01	0.00	0.00

Table S12. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **9**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.00											
2	C	0.01	0.00										
3	C	0.01	0.01	0.00									
4	Li	0.11	0.07	0.00	0.00								
5	Li	0.07	0.00	0.11	0.00	0.00							
6	Li	0.00	0.11	0.07	0.00	0.00	0.00						
7	C	2.99	0.01	0.01	0.01	0.06	0.00	0.00					
8	C	0.01	2.99	0.01	0.06	0.00	0.01	0.01	0.00				
9	C	0.01	0.01	2.99	0.00	0.01	0.06	0.01	0.01	0.00			
10	Li	0.00	0.06	0.01	0.00	0.00	0.01	0.00	0.07	0.11	0.00		
11	Li	0.06	0.01	0.00	0.01	0.00	0.00	0.07	0.11	0.00	0.00	0.00	
12	Li	0.01	0.00	0.06	0.00	0.01	0.00	0.11	0.00	0.07	0.00	0.00	0.00

Table S13. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **14**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.00											
2	C	0.04	0.00										
3	C	0.06	2.98	0.00									
4	C	0.04	0.01	0.01	0.00								
5	C	0.06	0.01	0.02	2.98	0.00							
6	C	0.01	0.01	0.01	0.01	0.01	0.00						
7	C	0.11	0.02	0.01	0.02	0.01	2.99	0.00					
8	Li	0.01	0.06	0.07	0.06	0.07	0.00	0.00	0.00				
9	Li	0.01	0.00	0.00	0.08	0.01	0.06	0.06	0.00	0.00			
10	Li	0.01	0.08	0.01	0.00	0.00	0.06	0.06	0.00	0.00	0.00		
11	Li	0.02	0.08	0.01	0.08	0.01	0.10	0.02	0.01	0.01	0.01	0.00	
12	Li	0.01	0.01	0.08	0.01	0.08	0.00	0.00	0.01	0.00	0.00	0.00	0.00

Table S14. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **13**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.00											
2	C	0.08	0.00										
3	C	0.08	2.97	0.00									
4	C	0.00	0.01	0.01	0.00								
5	C	0.00	0.01	0.01	2.99								
6	C	0.00	0.01	0.01	0.01	0.01	0.00						
7	C	0.00	0.01	0.01	0.01	0.01	2.99	0.00					
8	Li	0.00	0.01	0.09	0.07	0.07	0.00	0.00	0.00				
9	Li	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.00	0.00			
10	Li	0.00	0.09	0.01	0.00	0.00	0.07	0.07	0.00	0.00	0.00		
11	Li	0.00	0.03	0.03	0.09	0.01	0.09	0.01	0.01	0.01	0.01	0.00	
12	Li	0.00	0.03	0.03	0.01	0.09	0.01	0.09	0.01	0.01	0.01	0.01	0.00

Table S15. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **12**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.00											
2	C	0.08	0.00										
3	C	0.08	2.99	0.00									
4	C	0.00	0.01	0.01	0.00								
5	C	0.00	0.01	0.01	3.00	0.00							
6	C	0.00	0.01	0.01	0.01	0.01	0.00						
7	C	0.00	0.01	0.01	0.01	0.01	3.00	0.00					
8	Li	0.00	0.06	0.06	0.08	0.08	0.00	0.00	0.00				
9	Li	0.00	0.00	0.00	0.06	0.06	0.06	0.06	0.00	0.00			
10	Li	0.00	0.06	0.06	0.00	0.00	0.08	0.08	0.00	0.00	0.00		
11	Li	0.00	0.05	0.01	0.10	0.01	0.10	0.01	0.01	0.01	0.01	0.00	
12	Li	0.00	0.01	0.05	0.01	0.10	0.01	0.10	0.01	0.01	0.01	0.01	0.00

Table S16. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **11**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.00											
2	C	0.09											
3	C	0.09	2.99	0.00									
4	C	0.09	0.01	0.02	0.00								
5	C	0.09	0.02	0.01	2.99	0.00							
6	C	0.09	0.01	0.02	0.01	0.02	0.00						
7	C	0.09	0.02	0.01	0.02	0.01	2.99	0.00					
8	Li	0.02	0.05	0.05	0.05	0.05	0.00	0.00	0.00				
9	Li	0.02	0.00	0.00	0.05	0.05	0.05	0.05	0.00	0.00			
10	Li	0.02	0.05	0.05	0.00	0.00	0.05	0.05	0.00	0.00	0.00		
11	Li	0.03	0.05	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	
12	Li	0.03	0.00	0.05	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00

Table S17. Result of Wiberg bond indices at the ωB97XD/cc-pVQZ level for the structure **8**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.00											
2	C	1.44	0.00										
3	C	0.03	1.47	0.00									
4	C	0.12	0.03	1.44	0.00								
5	C	0.03	0.12	0.05	1.44	0.00							
6	C	1.44	0.05	0.12	0.03	1.47	0.00						
7	Li	0.03	0.15	0.15	0.03	0.01	0.01	0.00					
8	Li	0.01	0.03	0.16	0.15	0.03	0.01	0.01	0.00				
9	Li	0.01	0.01	0.03	0.15	0.16	0.03	0.00	0.01	0.00			
10	Li	0.03	0.01	0.01	0.03	0.15	0.15	0.00	0.00	0.01	0.00		
11	Li	0.15	0.03	0.01	0.01	0.03	0.16	0.00	0.00	0.00	0.01	0.00	
12	Li	0.15	0.16	0.03	0.01	0.01	0.03	0.01	0.00	0.00	0.00	0.01	0.00

Table S18. Result of Wiberg bond indices at the wb97XD/cc-pVQZ level for the structure **7**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.00											
2	C	1.46	0.00										
3	C	0.05	1.46	0.00									
4	C	0.14	0.05	1.46	0.00								
5	C	0.05	0.13	0.04	1.46	0.00							
6	C	1.46	0.04	0.13	0.05	1.46	0.00						
7	Li	0.03	0.03	0.01	0.03	0.03	0.42	0.00					
8	Li	0.42	0.03	0.03	0.01	0.03	0.03	0.02	0.00				
9	Li	0.03	0.42	0.03	0.03	0.01	0.03	0.02	0.02	0.00			
10	Li	0.03	0.03	0.42	0.03	0.03	0.01	0.02	0.02	0.02	0.00		
11	Li	0.01	0.03	0.03	0.42	0.03	0.03	0.02	0.02	0.02	0.02	0.00	
12	Li	0.03	0.01	0.03	0.03	0.42	0.03	0.02	0.02	0.02	0.02	0.02	0.00

Table S19. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure 10.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.000											
2	C	1.244	0.000										
3	C	4.036	3.550	0.000									
4	C	4.080	4.429	3.137	0.000								
5	C	3.555	3.145	1.245	3.619	0.000							
6	C	3.361	4.025	3.690	1.244	3.795	0.000						
7	Li	2.203	2.218	2.376	2.253	2.548	2.181	0.000					
8	Li	2.058	3.182	4.648	3.194	4.347	2.057	2.561	0.000				
9	Li	4.894	4.708	2.087	2.034	3.153	3.148	2.712	4.778	0.000			
10	Li	2.191	2.108	3.126	4.367	2.086	3.916	2.753	3.409	4.701	0.000		
11	Li	3.890	4.123	2.309	2.097	2.178	2.238	2.527	3.525	2.633	3.101	0.000	
12	Li	3.111	2.035	2.326	4.566	2.212	4.681	2.596	4.666	3.946	2.586	3.973	0.000

Table S20. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure 15.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.000											
2	C	2.095	0.000										
3	C	2.291	1.244	0.000									
4	C	2.291	4.113	4.570	0.000								
5	C	2.095	3.389	4.113	1.244	0.000							
6	C	2.295	4.043	3.554	3.139	3.720	0.000						
7	C	2.295	3.720	3.139	3.554	4.043	1.246	0.000					
8	Li	2.424	2.072	3.214	3.214	2.072	4.675	4.675	0.000				
9	Li	2.582	4.538	4.557	2.020	3.024	2.242	2.268	4.478	0.000			
10	Li	2.582	3.024	2.020	4.557	4.538	2.268	2.242	4.478	4.130	0.000		
11	Li	2.571	4.495	4.503	2.037	2.653	2.104	3.149	4.202	2.550	3.667	0.000	
12	Li	2.571	2.653	2.037	4.503	4.495	3.149	2.104	4.202	3.667	2.550	4.680	0.000

Table S21. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **9**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.000											
2	C	3.669	0.000										
3	C	3.669	3.669	0.000									
4	Li	2.056	2.179	4.000	0.000								
5	Li	2.179	4.000	2.056	3.139	0.000							
6	Li	4.000	2.056	2.179	3.139	3.139	0.000						
7	C	1.244	4.115	3.344	3.041	2.195	4.230	0.000					
8	C	3.344	1.244	4.115	2.195	4.230	3.041	3.669	0.000				
9	C	4.115	3.344	1.244	4.230	3.041	2.195	3.669	3.669	0.000			
10	Li	4.230	2.195	3.041	3.738	4.165	2.500	4.000	2.179	2.056	0.000		
11	Li	2.195	3.041	4.230	2.500	3.738	4.165	2.179	2.056	4.000	3.139	0.000	
12	Li	3.041	4.230	2.195	4.165	2.500	3.738	2.056	4.000	2.179	3.139	3.139	0.000

Table S22. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **14**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.000											
2	C	2.363	0.000										
3	C	2.303	1.244	0.000									
4	C	2.363	3.411	3.462	0.000								
5	C	2.303	3.462	3.061	1.244	0.000							
6	C	2.910	3.499	4.368	3.499	4.368	0.000						
7	C	2.046	3.311	3.890	3.311	3.890	1.246	0.000					
8	Li	2.881	2.241	2.116	2.241	2.116	4.402	4.291	0.000				
9	Li	2.703	4.207	4.623	2.110	3.079	2.213	2.160	4.015	0.000			
10	Li	2.703	2.110	3.079	4.207	4.623	2.213	2.160	4.015	3.885	0.000		
11	Li	2.464	2.250	3.102	2.250	3.102	2.052	2.454	2.497	2.459	2.459	0.000	
12	Li	2.594	3.149	2.086	3.149	2.086	5.348	4.634	2.485	4.708	4.708	4.111	0.000

Table S23. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **13**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.000											
2	C	2.043	0.000										
3	C	2.043	1.246	0.000									
4	C	5.401	3.962	3.380	0.000								
5	C	5.401	3.962	3.380	1.246	0.000							
6	C	5.401	3.380	3.962	3.435	3.654	0.000						
7	C	5.401	3.380	3.962	3.654	3.435	1.246	0.000					
8	Li	3.921	3.184	2.088	2.109	2.109	4.516	4.516	0.000				
9	Li	6.313	4.411	4.411	2.203	2.203	2.203	2.203	3.915	0.000			
10	Li	3.921	2.088	3.184	4.516	4.516	2.109	2.109	4.642	3.915	0.000		
11	Li	4.299	2.596	2.596	2.104	2.781	2.104	2.781	2.830	2.588	2.830	0.000	
12	Li	4.299	2.596	2.596	2.781	2.104	2.781	2.104	2.830	2.588	2.830	2.651	0.000

Table S24. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **12**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.000											
2	C	2.059	0.000										
3	C	2.059	1.249	0.000									
4	C	5.374	3.534	3.748	0.000								
5	C	5.374	3.748	3.534	1.245	0.000							
6	C	5.374	3.534	3.748	3.409	3.629	0.000						
7	C	5.374	3.748	3.534	3.629	3.409	1.245	0.000					
8	Li	3.606	2.286	2.286	2.101	2.101	4.171	4.171	0.000				
9	Li	6.290	4.373	4.373	2.193	2.193	2.193	2.193	3.748	0.000			
10	Li	3.606	2.286	2.286	4.171	4.171	2.101	2.101	3.809	3.748	0.000		
11	Li	4.496	2.440	3.131	2.108	2.878	2.108	2.878	2.711	2.577	2.711	0.000	
12	Li	4.496	3.131	2.440	2.878	2.108	2.878	2.108	2.711	2.577	2.711	3.081	0.000

Table S25. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **11**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	Li	0.000											
2	C	2.031	0.000										
3	C	2.031	1.247	0.000									
4	C	2.031	3.348	3.573	0.000								
5	C	2.031	3.573	3.348	1.247	0.000							
6	C	2.031	3.348	3.573	3.348	3.573	0.000						
7	C	2.031	3.573	3.348	3.573	3.348	1.247	0.000					
8	Li	2.302	2.231	2.231	2.231	2.231	4.281	4.281	0.000				
9	Li	2.302	4.281	4.281	2.231	2.231	2.231	2.231	3.988	0.000			
10	Li	2.302	2.231	2.231	4.281	4.281	2.231	2.231	3.988	3.988	0.000		
11	Li	2.067	2.413	3.313	2.413	3.313	2.413	3.313	3.094	3.094	3.094	0.000	
12	Li	2.067	3.313	2.413	3.313	2.413	3.313	2.413	3.094	3.094	3.094	4.135	0.000

Table S26. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **8**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.000											
2	C	1.414	0.000										
3	C	2.448	1.414	0.000									
4	C	2.827	2.448	1.414	0.000								
5	C	2.448	2.827	2.448	1.414	0.000							
6	C	1.414	2.448	2.827	2.448	1.414	0.000						
7	Li	3.317	1.912	1.912	3.317	4.283	4.283	0.000					
8	Li	4.283	3.317	1.912	1.912	3.317	4.283	3.000	0.000				
9	Li	4.283	4.283	3.317	1.912	1.912	3.317	5.197	3.000	0.000			
10	Li	3.317	4.283	4.283	3.317	1.912	1.912	6.001	5.197	3.000	0.000		
11	Li	1.912	3.317	4.283	4.283	3.317	1.912	5.197	6.001	5.197	3.000	0.000	
12	Li	1.912	1.912	3.317	4.283	4.283	3.317	3.000	5.197	6.001	5.197	3.000	0.000

Table S27. Result of distance matrix (Å) at the ωB97XD/cc-pVQZ level for the structure **7**.

	Atom	1	2	3	4	5	6	7	8	9	10	11	12
1	C	0.000											
2	C	1.414	0.000										
3	C	2.448	1.414	0.000									
4	C	2.827	2.448	1.414	0.000								
5	C	2.448	2.827	2.448	1.414	0.000							
6	C	1.414	2.448	2.827	2.448	1.414	0.000						
7	Li	2.004	2.975	4.303	4.832	4.303	2.975	0.000					
8	Li	2.975	2.004	2.975	4.303	4.832	4.303	3.418	0.000				
9	Li	4.303	2.975	2.004	2.975	4.303	4.832	5.920	3.418	0.000			
10	Li	4.832	4.303	2.975	2.004	2.975	4.303	6.836	5.920	3.418	0.000		
11	Li	4.303	4.832	4.303	2.975	2.004	2.975	5.920	6.836	5.920	3.418	0.000	
12	Li	2.975	4.303	4.832	4.303	2.975	2.004	3.418	5.920	6.836	5.920	3.418	0.000

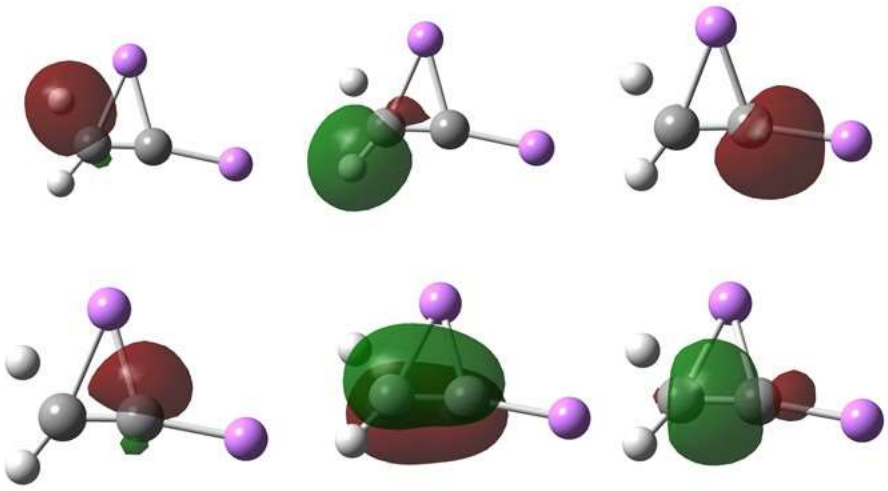

Figure S1. Localized molecular orbitals of structure **1.**

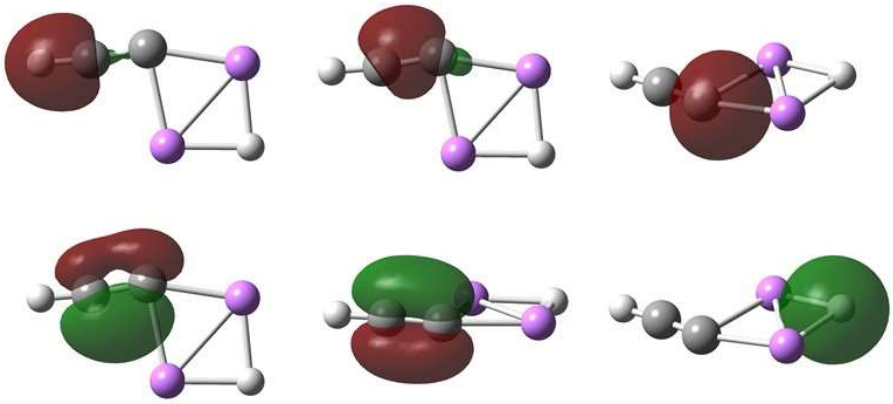

Figure S2. Localized molecular orbitals of structure **2**.

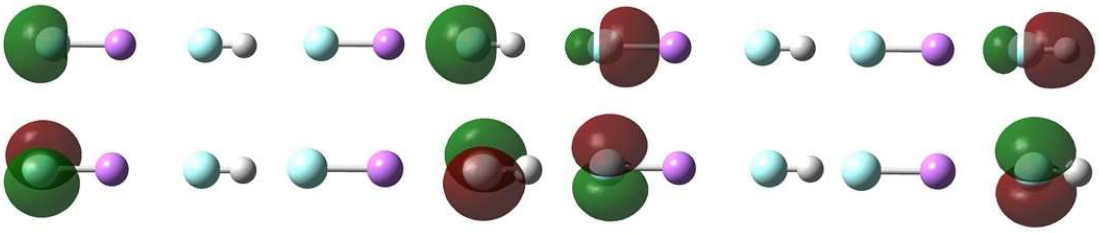

Figure S3. Localized molecular orbitals of structure **3**.

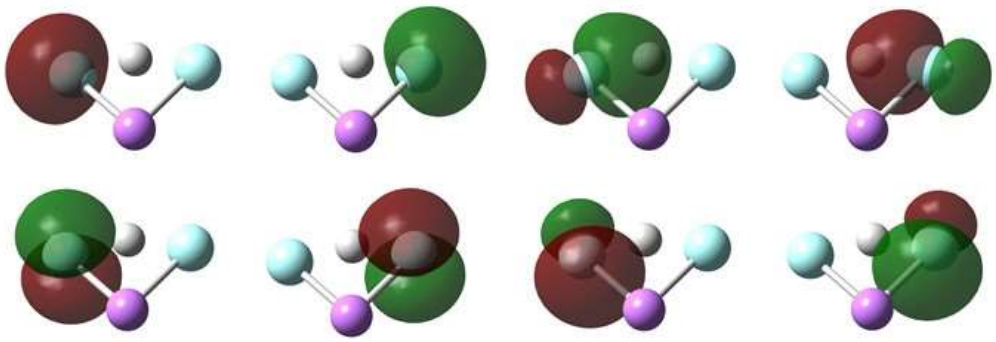

Figure S4. Localized molecular orbitals of structure **4**.

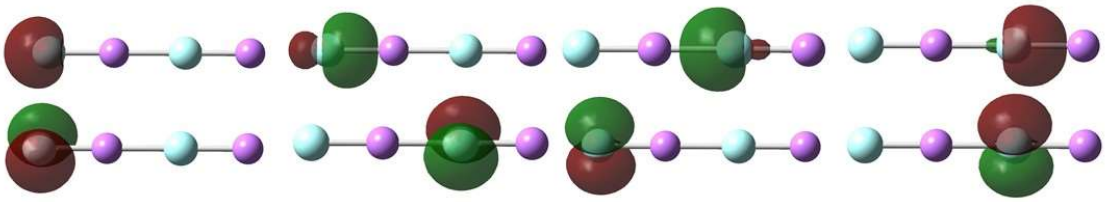

Figure S5. Localized molecular orbitals of structure **5**.

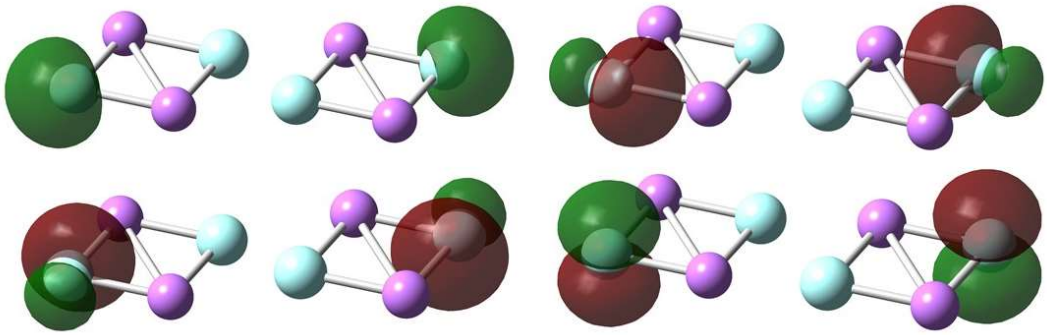

Figure S6. Localized molecular orbitals of structure **6**.

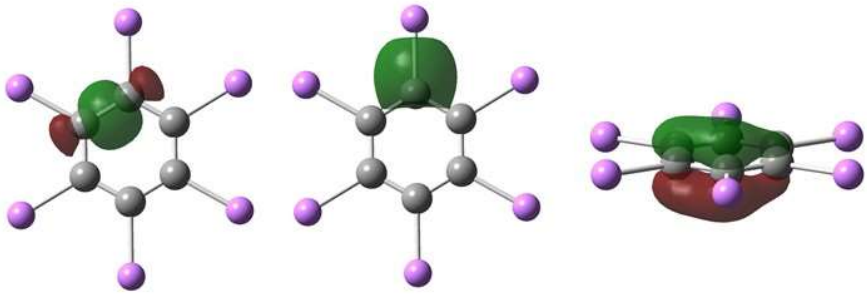

Figure S7. Localized molecular orbitals of structure **7**.

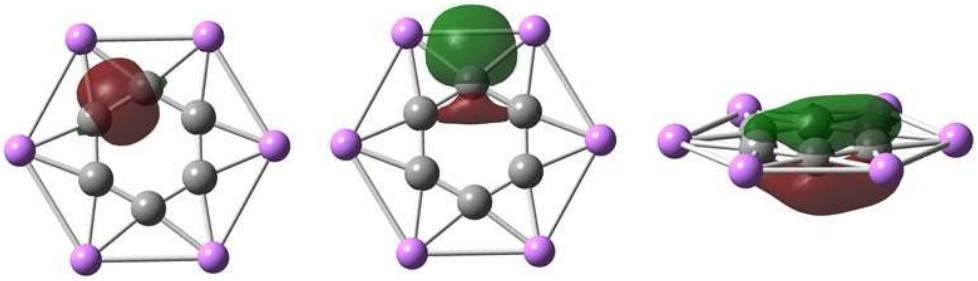

Figure S8. Localized molecular orbitals of structure **8**.

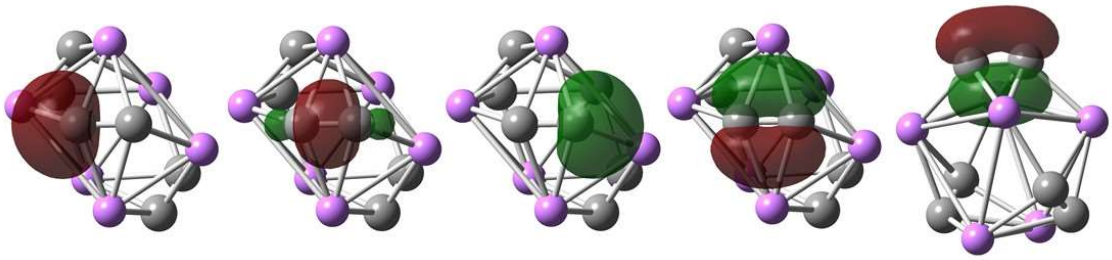

Figure S9. Localized molecular orbitals of structure **9**.

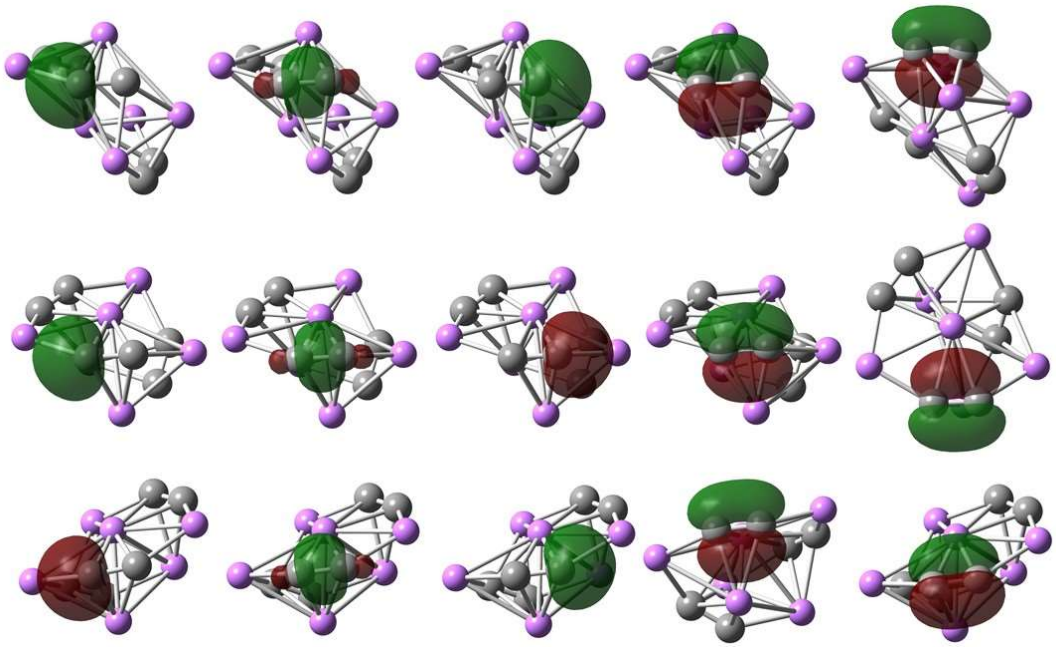

Figure S10. Localized molecular orbitals of structure **10**.

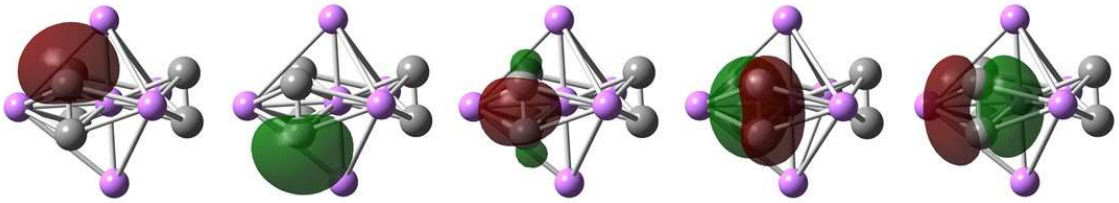

Figure S11. Localized molecular orbitals of structure **11**.

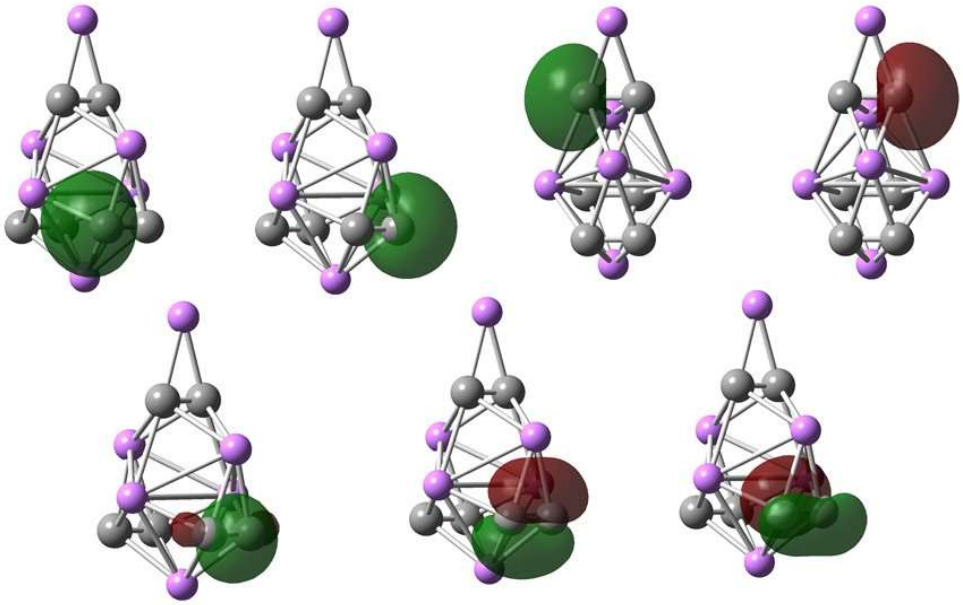

Figure S12. Localized molecular orbitals of structure **12**.

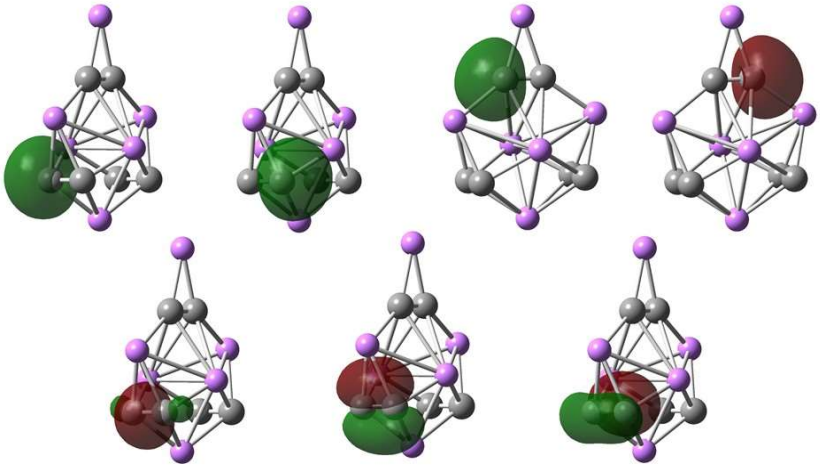

Figure S13. Localized molecular orbitals of structure **13**.

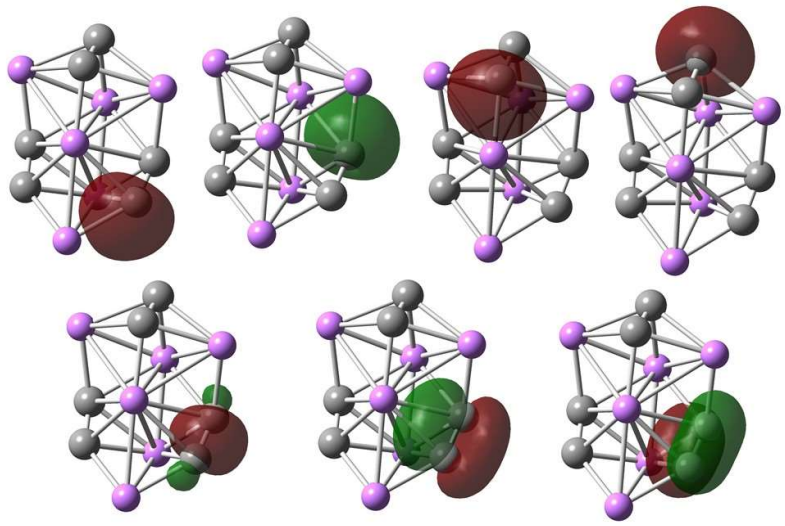

Figure S14. Localized molecular orbitals of structure **14**.

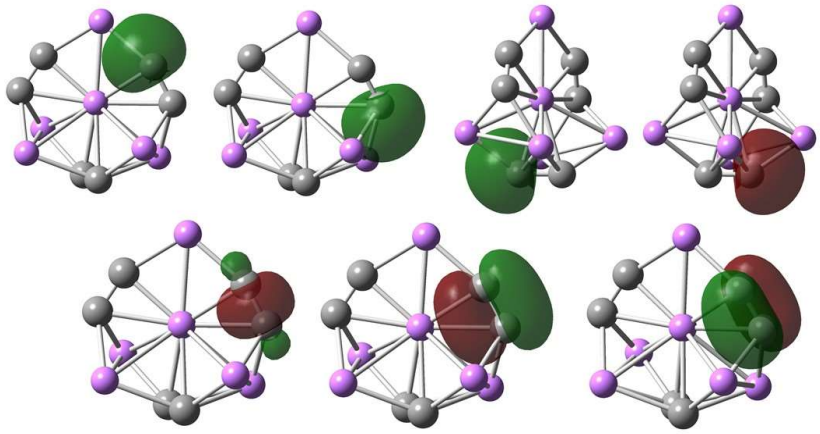

Figure S15. Localized molecular orbitals of structure **15.**