Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPORTING INFORMATION

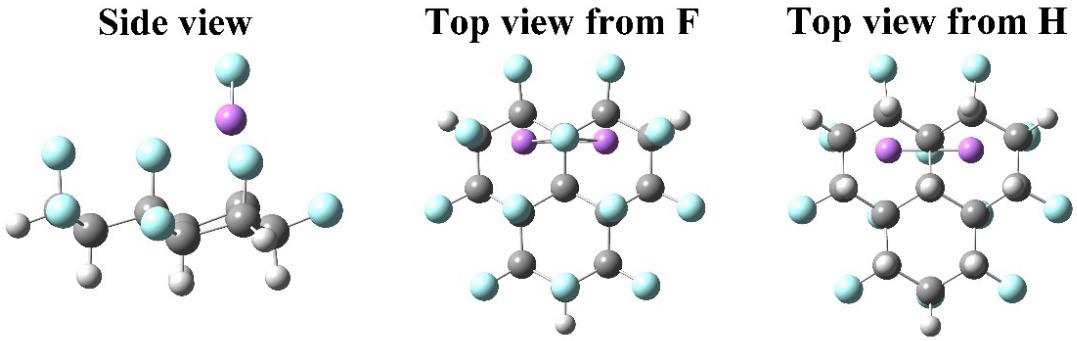

Figure S1 Optimized structures of the 2Li-**1** system.

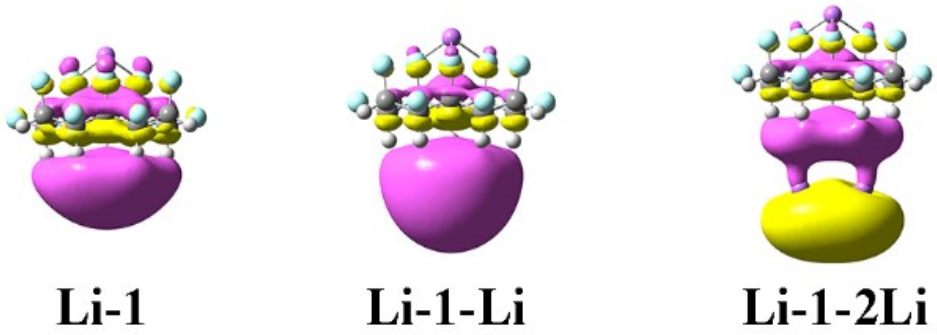

Figure S2 The highest occupied molecular orbitals (HOMOs) of the Li-**1**-nLi (n=0,1,2) compounds.

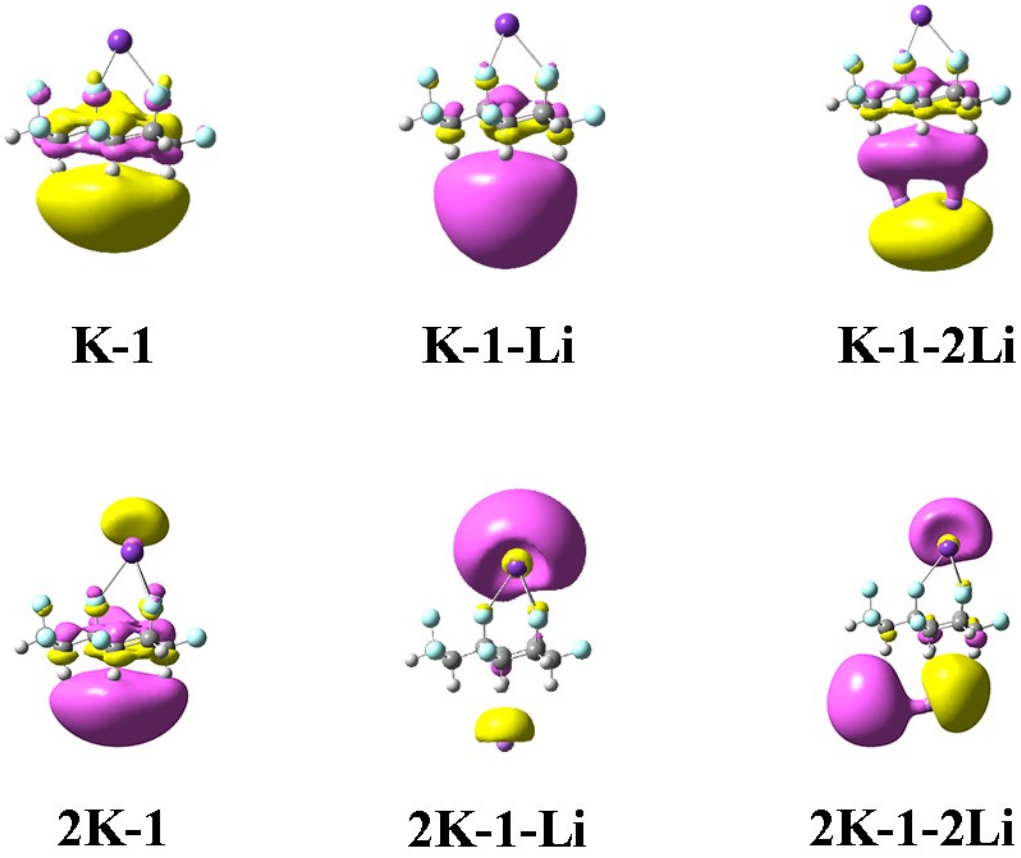

Figure S3 The highest occupied molecular orbitals (HOMOs) of the mK-**1**-nLi (m=1,2; n=0,1,2) compounds.

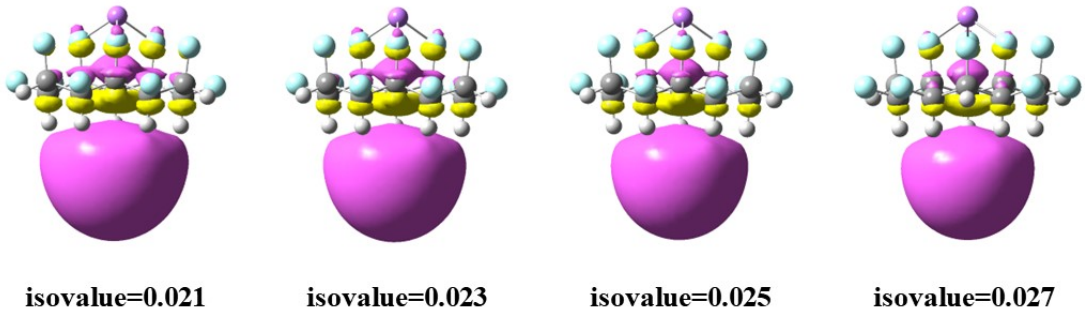

Figure S4 The HOMO of the Li-**1**-Li compound.

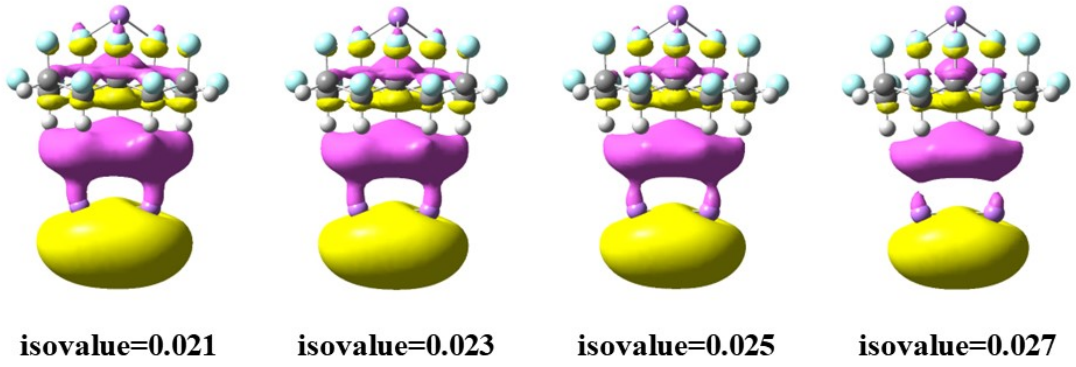

Figure S5 The HOMO of the Li-**1**-2Li compound.

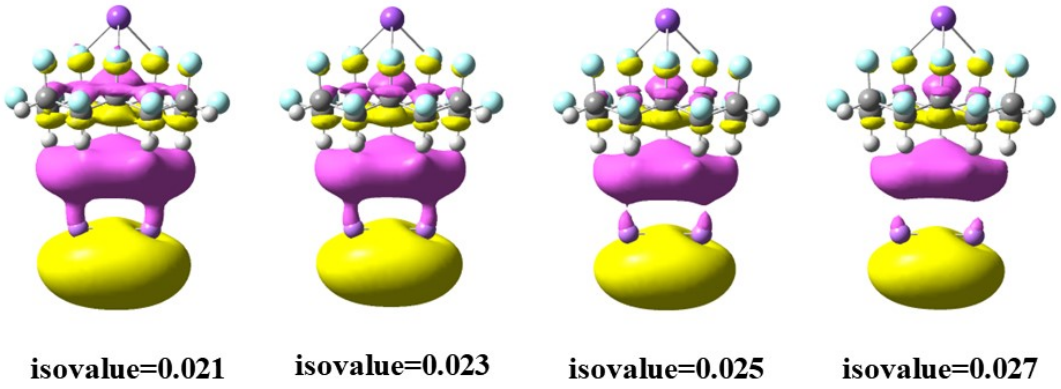

Figure S6 The HOMO of the Na-**1**-2Li compound.

Table S1 The first hyperpolarizability (β_0, in au) of the Li-$F_6C_6H_6$ system is calculated by the **LC-tHCTH**, **wb97x**, **wb97xd** and **M11** method with different basis sets.

Basis sets	LC-tHCTH	wb97x	wb97xd	M11
6-31G	165401	124695	53735	96044
6-31G(d)	112886	69674	60582	53591
6-31+G(d)	751879	487654	214623	84071
6-31+G(d, p)	761595	513811	225164	89209
6-31++G(d, p)	766493	**695952**	355695	123341
6-311+G(d)	743688	**691799**	311039	136206
6-311+G(d, p)	734650	**698235**	307644	141028
6-311++G(d, p)	718381	981632	483811	165808
6-311++G(2d, 2p)	472783	502871	250376	71778
6-311++G(3df,3pd)	1371794	558487	326106	44972

Table S2 The first hyperpolarizability (β_0, in au) of the Li-**1** system is calculated by the **wb97x** method with different basis sets.

Basis sets	β_0
6-31++G(d, p)	**16030**
6-311+G(d)	4770
6-311+G(d, p)	4486

Table S3 Energy calculations of the different spin states of mM$_F$-**1**-nLi compounds.

	singlet	***triplet***	***quintet***	***doublet***	***quartet***
Li-1-Li	-1713.983932	-1713.939962			
Na-1-Li	-1868.719049	-1868.675334			
K-1-Li	-2306.352663	-2306.308657			
Li-1-2Li				-1721.467622	-1721.428465
Na-1-2Li				-1876.202782	-1876.164361
K-1-2Li				-2313.836559	-2313.798634
2Na-1	-2023.449447	-2023.445493			
2K-1	-2898.699215	-2898.700079			
2Na-1-Li				-2030.977592	-2030.927304
2K-1-Li				-2906.230482	-2906.182238
2Na-1-2Li	-2038.464404	-2038.477452	-2038.418223		
2K-1-2Li	-2913.716298	-2913.731076	-2913.673185		