External Electric Field Driven Configurations Transition between Lithium Salt and Electride-like Molecule: Intriguing NLO Switches in Li@Corannulene

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Table of contents

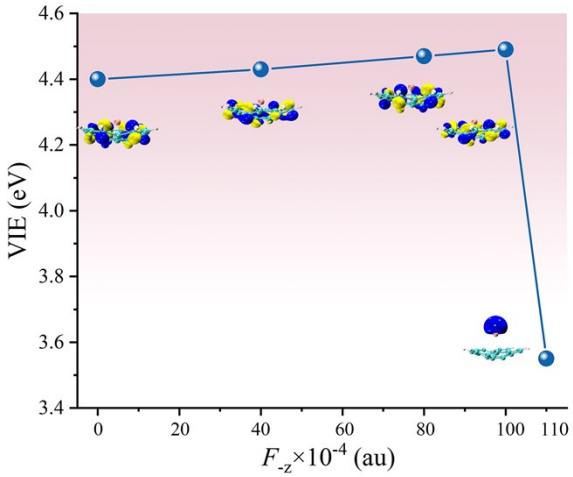

Figure S1. Evolutions of the vertical ionisation energy (VIE) value of the Li@corannulene under the vertical F_{-z} (F_{-z} = 1×10^{-4}, au)

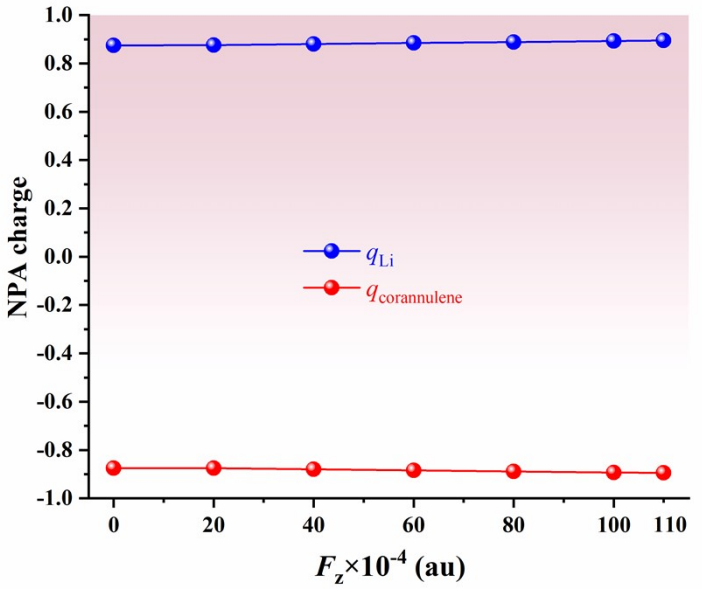

Figure S2. Evolutions of the natural population analysis (NPA) charges of the Li@corannulene under the vertical F_z ($F_z = 1\times10^{-4}$, au)

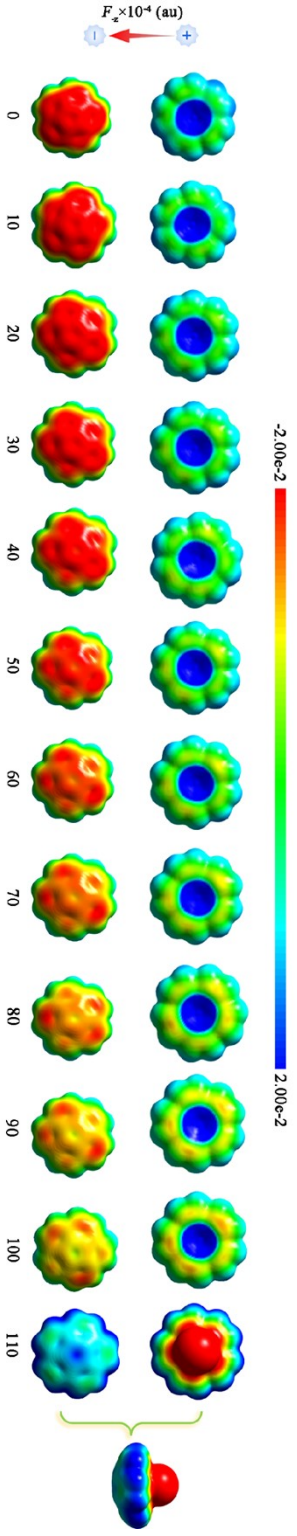

Figure S3. Electrostatic potential maps (ESP) of the Li@corannulene with allelic values of ± 2.00 e^{-2} au under the vertical F_{-z} ($F_{-z} = 1\times10^{-4}$, au)

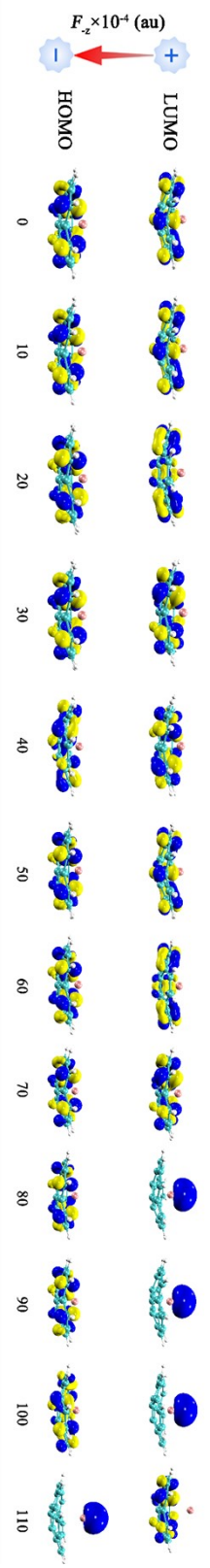

Figure S4. Evolutions of the frontier molecular orbitals of the Li@corannulene under the vertical F_{-z} (F_{-z} = 1×10^{-4}, au)

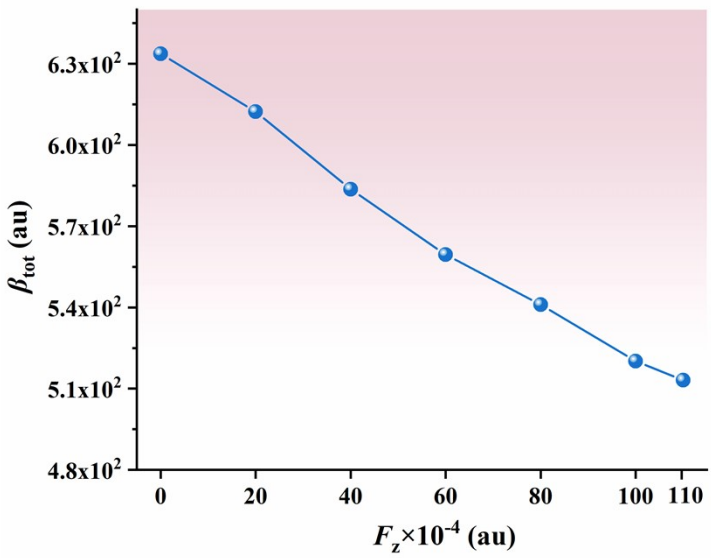

Figure S5. Evolutions of the first hyperpolarizabilities (β_{tot}) of Li@corannulene under the vertical F_z ($F_z = 1\times10^{-4}$, au)

Table S1. Evolutions of the bond length alternation (BLA) of Li@corannulene under the vertical F_z ($F_z = 1\times10^{-4}$, au)

$F_{-z} = 1\times10^{-4}$ (au)	BLA (Angstrom)
0	0.01
40	0.01
80	0.02
100	0.02
110	0.00

Cartesian Coordinates of the optimized structures ($F_{\pm z}$ =0, au)

Li@corannulene	The total energy = -775.695 au		
Atom	**X**	**Y**	**Z**
C	0.83324	-3.18907	-0.19262
C	-0.54986	-3.25038	-0.19229
H	-1.02243	-4.17466	-0.51877
C	-1.39563	-2.09926	0.1229
C	-2.7755	-1.77794	-0.19262
H	-3.37495	-2.57389	-0.63723
C	-3.26121	-0.48148	-0.19229
H	-4.28629	-0.31765	-0.51877
C	-2.42779	0.67862	0.1229
C	-2.54859	2.09024	-0.19262
H	-3.49083	2.41439	-0.63723
C	-1.46568	2.95281	-0.19229
H	-1.62664	3.97834	-0.51877
C	-0.10483	2.51867	0.1229
C	1.20038	3.06978	-0.19262
H	1.21749	4.06606	-0.63723
C	2.35537	2.30641	-0.19229
H	3.28097	2.7764	-0.51877
C	2.363	0.87801	0.1229
C	3.29047	-0.19302	-0.19262
H	4.24328	0.09858	-0.63723
C	2.92138	-1.52736	-0.19229
H	3.65439	-2.26243	-0.51877
C	1.56524	-1.97603	0.1229
C	0.74706	-0.95024	0.64433
C	1.13458	0.41685	0.64433
C	-0.04585	1.20787	0.64433
C	-1.16292	0.32965	0.64433
C	-0.67288	-1.00413	0.64433
H	1.405	-4.00514	-0.63723
Li	0.000	0. 000	-1.17665