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Electronic Supplementary Information (ESI) for

Bowl-Shaped Carbon Skeleton under Tensile Stress: Quantum Mechanochemistry of Corannulene

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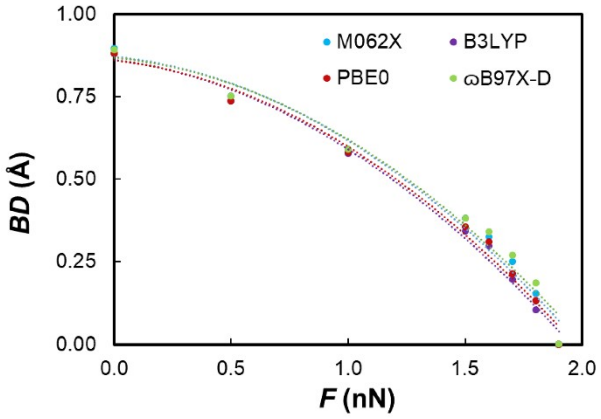

Fig. S1. Correlations and fitting curves (in dashed lines) between applied force (*F*) and bowl-depth (*BD*) of COR stretching using different density functionals.

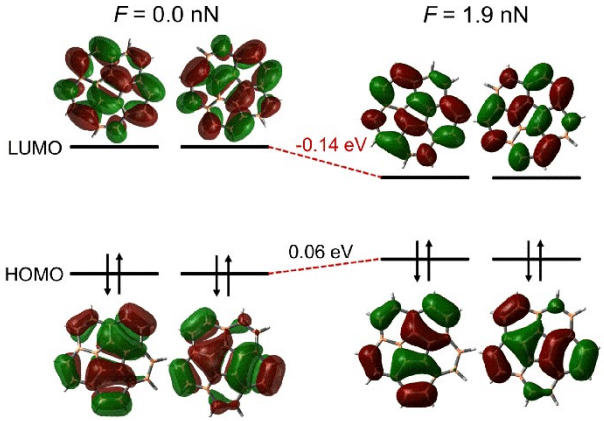

Fig. S2. Frontier orbital diagrams (isovalue = 0.02 au) and energy levels of COR at *F* = 0.0 nN and *F* = 1.9 nN.

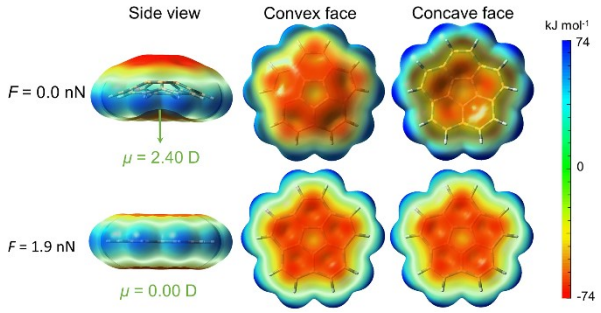

Fig. S3. Electrostatic potential maps of COR at *F* = 0.0 and *F* = 1.9 nN

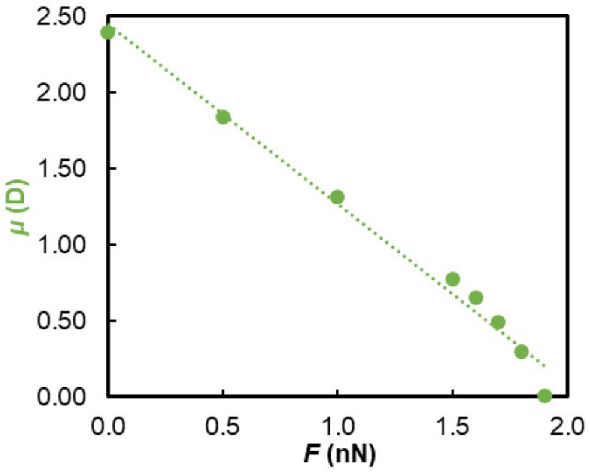

Fig. S4. Correlation and fitting curve (in dashed line) between applied force (F) and dipole moment (μ) of COR.

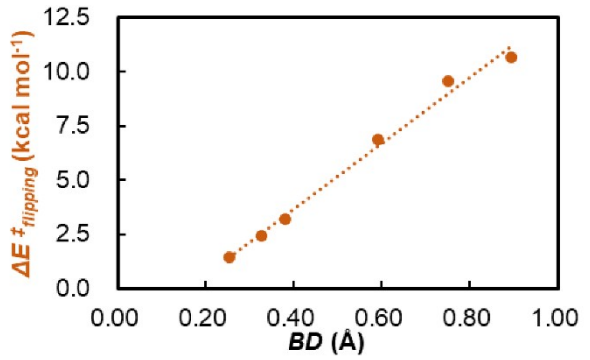

Fig. S5. Correlation and fitting curve (in dashed line) between bowl-depth (BD) of COR and reaction barrier of corannulene flipping.

Table S1. Calculated bowl-depths (BD) and electronic energies (E) of COR under applied forces (F).

F (nN)	BD (Å)	E (a.u.)
0.0	0.895	-768.0093
0.5	0.751	-768.0072
1.0	0.591	-768.0018
1.5	0.381	-767.9941
1.6	0.327	-767.9923
1.7	0.252	-767.9903
1.8	0.155	-767.9884
1.9	0.000	-767.9869

Table S2. Calculated bond lengths of COR under applied forces (*F*).

F (nN)	bond length (Å)				
	hub	spoke	flank	rim	C-H
0.0	1.416	1.376	1.445	1.379	1.085
0.5	1.413	1.373	1.453	1.385	1.089
1.0	1.411	1.371	1.462	1.391	1.093
1.5	1.409	1.369	1.470	1.398	1.098
1.6	1.408	1.368	1.472	1.399	1.099
1.7	1.408	1.368	1.474	1.400	1.100
1.8	1.407	1.368	1.476	1.401	1.101
1.9	1.407	1.367	1.477	1.402	1.102

Table S3. Calculated bond lengths of the transition states of COR flipping under applied forces (*F*).

F (nN)	bond length of TS (Å)				
	hub	spoke	flank	rim	C-H
0.0	1.396	1.359	1.461	1.394	1.085
0.5	1.399	1.361	1.465	1.396	1.089
1.0	1.402	1.363	1.469	1.398	1.093
1.5	1.405	1.366	1.474	1.400	1.098
1.6	1.406	1.366	1.475	1.400	1.099
1.7	1.406	1.367	1.476	1.401	1.100
1.8	1.407	1.367	1.476	1.401	1.101

Table S4. Calculated bowl-depths (*BD*) of COR under applied forces (*F*) using different density functionals.

F (nN)	*BD* (Å)			
	M062X	B3LYP	PBE0	ωB97X-D
0.0	0.895	0.882	0.881	0.892
0.5	0.751	0.736	0.737	0.752
1.0	0.591	0.578	0.583	0.591
1.5	0.381	0.344	0.356	0.382
1.6	0.327	0.299	0.310	0.342
1.7	0.252	0.197	0.214	0.271
1.8	0.155	0.105	0.134	0.187
1.9	0.000	0.003	0.000	0.001

Table S5. Calculated bowl-depths (*BD*) of COR derivatives under applied forces (*F*).

F (nN)	*BD* (Å)		
	$C_{20}F_{10}$	$C_{20}Cl_{10}$	$C_{20}H_{10}$
0.0	0.870	0.553	0.895
0.5	0.711	0.394	0.751
1.0	0.538	0.000	0.591
1.5	0.316	-	0.381
1.6	0.236	-	0.327
1.7	0.087	-	0.252
1.8	0.015	-	0.155
1.9	0.007	-	0.000

Table S6. Calculated frontier orbital energy levels of COR at $F = 0.0$ and $F = 1.9$ nN.

F (nN)	LUMO energy (eV)	HOMO energy (eV)
0.0	-1.07	-7.55
1.9	-1.21	-7.49

Table S7. Calculated NICS vales of the centers of hub pentagon ($NICS_p$) and hexagon ($NICS_h$) of COR under stress.

F (nN)	$NICS_p$	$NICS_h$
0.0	8.95	-6.60
0.5	10.17	-6.01
1.0	10.96	-5.56
1.5	11.42	-5.21
1.9	11.54	-5.01

Table S8. Calculated dipole moments (μ) of COR under applied forces (*F*).

F (nN)	μ (D)
0.0	2.395
0.5	1.835
1.0	1.314
1.5	0.772
1.6	0.650
1.7	0.490
1.8	0.298
1.9	0.003

Table S9. Calculated energies of reactant (E_{COR}) and transition state (E_{TS}) for COR flipping under applied forces (F).

F (nN)	E_{COR} (a.u.)	E_{TS} (a.u.)
0.0	-768.0093	-767.9923
0.5	-768.0072	-767.9919
1.0	-768.0018	-767.9908
1.5	-767.9941	-767.9890
1.6	-767.9923	-767.9885
1.7	-767.9903	-767.9880
1.8	-767.9884	-767.9883

Table S10. Calculated binding energy of C_{60}@COR (E_{bind}) under applied forces (F).

F (nN)	E_{bind} (a.u.)
0.0	-3053.9193
0.5	-3053.9181
1.0	-3053.9139
1.5	-3053.9077
1.6	-3053.9068
1.7	-3053.9058
1.8	-3053.9040
1.9	-3053.9032