Theoretical study on the relationship between the molecular structures and optoelectronic properties of aromatic-fluorinated sumanene derivatives

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Table S1. Main geometric parameters of sumanene and its aromatic-fluorinated derivatives at the ground state. (Unit: Å)

Molecules	rimC-C (r1/r2/r3)			vertexC-C (v1/v2/…/v6)						rim-quatC=C (rq1/rq2/…/rq6)					
0	1.431	1.431	1.431	1.555	1.555	1.555	1.555	1.555	1.555	1.400	1.400	1.400	1.400	1.400	1.400
1	1.425	1.431	1.431	1.554	1.555	1.555	1.555	1.555	1.550	1.393	1.398	1.399	1.400	1.400	1.400
2	1.433	1.431	1.431	1.549	1.555	1.555	1.555	1.555	1.549	1.390	1.390	1.399	1.399	1.399	1.399
3	1.425	1.425	1.431	1.554	1.550	1.554	1.555	1.555	1.549	1.393	1.398	1.393	1.398	1.399	1.399
4	1.425	1.425	1.431	1.554	1.554	1.549	1.555	1.555	1.549	1.393	1.398	1.398	1.393	1.400	1.400
5	1.425	1.431	1.425	1.554	1.555	1.555	1.554	1.549	1.549	1.393	1.398	1.399	1.399	1.398	1.393
6	1.433	1.425	1.431	1.549	1.549	1.554	1.555	1.555	1.549	1.390	1.390	1.393	1.398	1.399	1.399
7	1.433	1.425	1.431	1.549	1.554	1.549	1.555	1.555	1.549	1.390	1.390	1.398	1.393	1.399	1.399
8	1.425	1.425	1.425	1.554	1.549	1.554	1.549	1.554	1.549	1.393	1.398	1.393	1.398	1.393	1.398
9	1.425	1.425	1.425	1.554	1.549	1.554	1.554	1.549	1.549	1.393	1.398	1.393	1.398	1.398	1.393
10	1.433	1.433	1.431	1.549	1.549	1.549	1.555	1.555	1.549	1.390	1.390	1.390	1.390	1.399	1.399
11	1.433	1.425	1.425	1.549	1.549	1.554	1.549	1.554	1.549	1.390	1.390	1.393	1.397	1.393	1.397
12	1.433	1.425	1.425	1.549	1.549	1.554	1.554	1.549	1.549	1.390	1.390	1.393	1.397	1.397	1.393
13	1.433	1.425	1.425	1.549	1.554	1.549	1.549	1.554	1.549	1.390	1.390	1.397	1.393	1.393	1.397
14	1.433	1.433	1.425	1.549	1.549	1.549	1.549	1.554	1.549	1.390	1.390	1.390	1.390	1.393	1.397
15	1.433	1.433	1.433	1.549	1.549	1.549	1.549	1.549	1.549	1.390	1.390	1.390	1.390	1.390	1.390

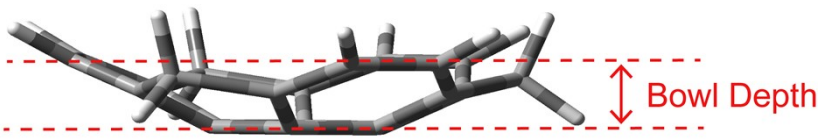


Figure S1. Graphical representation of the molecular bowl depth which is the average value of the vertical distance of the rim carbons and the hub carbons of the sumanene skeleton. (take sumanene as an example.)

Table S2. HOMO, LUMO energy levels, HOMO-LUMO energy gap (Δ H-L) and the lowest excitation energy (E_g) of sumanene and its aromatic-fluorinated derivatives. (Units: eV)

Molecules	HOMO	LUMO	ΔH-L	E_g
0	-5.48	-0.73	4.75	3.86
1	-5.51	-0.92	4.60	3.83
2	-5.60	-0.98	4.62	3.83
3	-5.60	-1.02	4.59	3.83
4	-5.54	-1.03	4.52	3.80
5	-5.59	-1.10	4.49	3.79
6	-5.73	-1.14	4.59	3.81
7	-5.64	-1.11	4.53	3.80
8	-5.76	-1.10	4.66	3.83
9	-5.64	-1.20	4.44	3.77
10	-5.77	-1.21	4.56	3.81
11	-5.77	-1.24	4.52	3.80
12	-5.75	-1.26	4.50	3.79
13	-5.71	-1.29	4.42	3.75
14	-5.84	-1.34	4.50	3.78
15	-5.98	-1.43	4.55	3.76

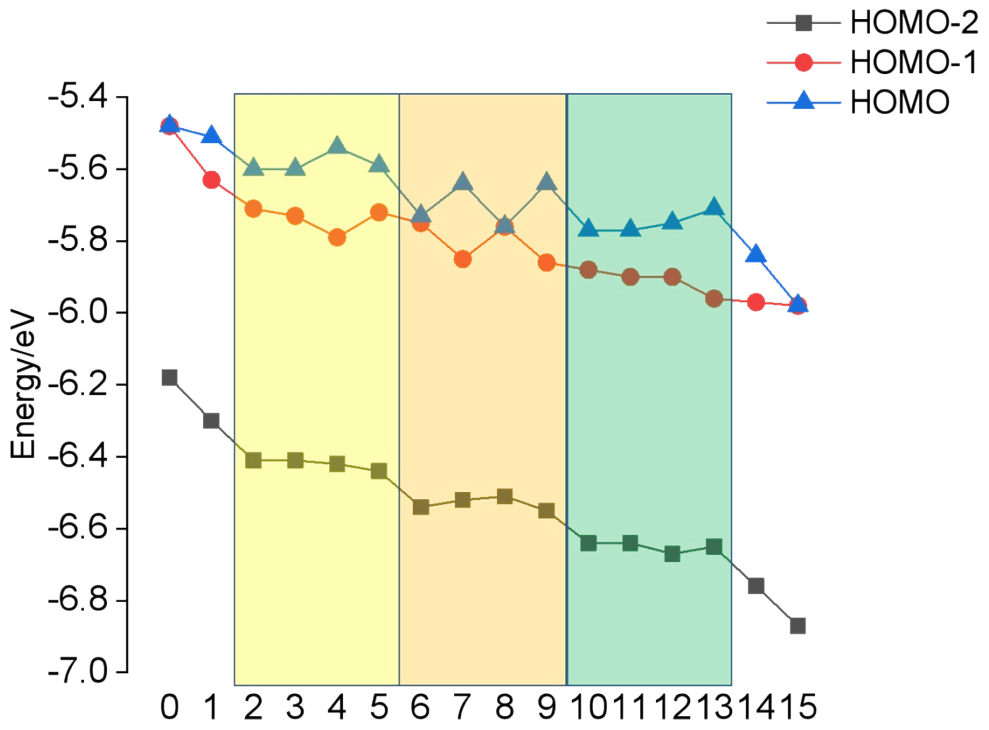


Figure S2. HOMO, HOMO-1 and HOMO-2 energy levels of sumanene and its aromatic-fluorinated derivatives. The values of disubstituted, trisubstituted and tetrasubstituted sumanene derivatives were painted on yellow, orange and green backgrounds respectively.

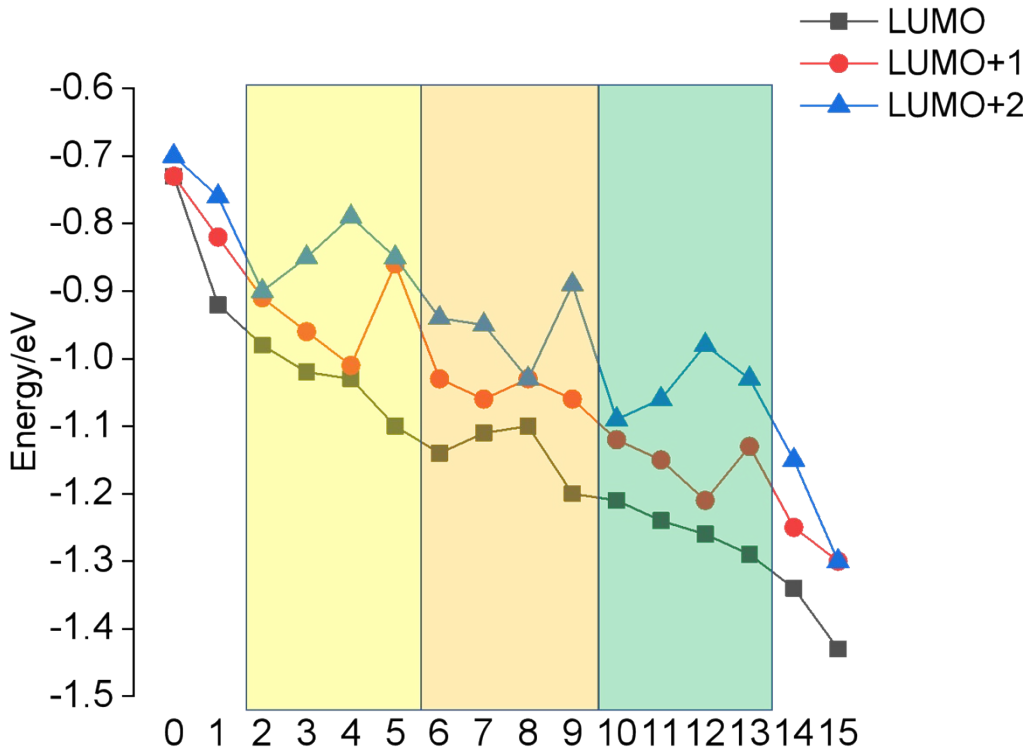
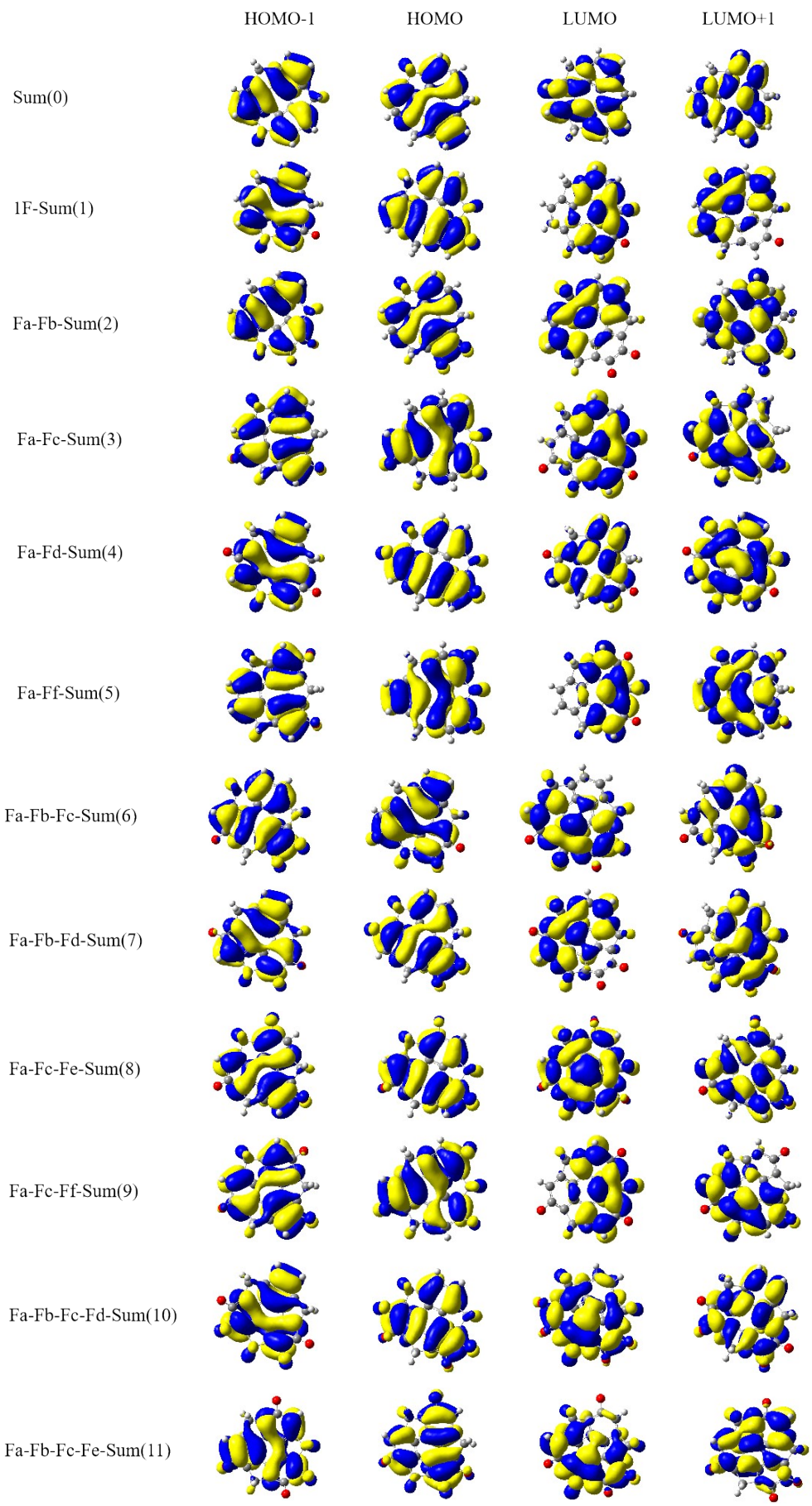


Figure S3. LUMO, LUMO+1 and LUMO+2 energy levels of sumanene and its aromatic-fluorinated derivatives. The values of disubstituted, trisubstituted and tetrasubstituted sumanene derivatives were painted on yellow, orange and green backgrounds respectively.


HOMO-1
HOMO
LUMO
LUMO+1
Sum(0)
1F-Sum(1)
Fa-Fb-Sum(2)
Fa-Fc-Sum(3)
Fa-Fd-Sum(4)
Fa-Ff-Sum(5)
Fa-Fb-Fc-Sum(6)
Fa-Fb-Fd-Sum(7)
Fa-Fc-Fe-Sum(8)
Fa-Fc-Ff-Sum(9)
Fa-Fb-Fc-Fd-Sum(10)
Fa-Fb-Fc-Fe-Sum(11)

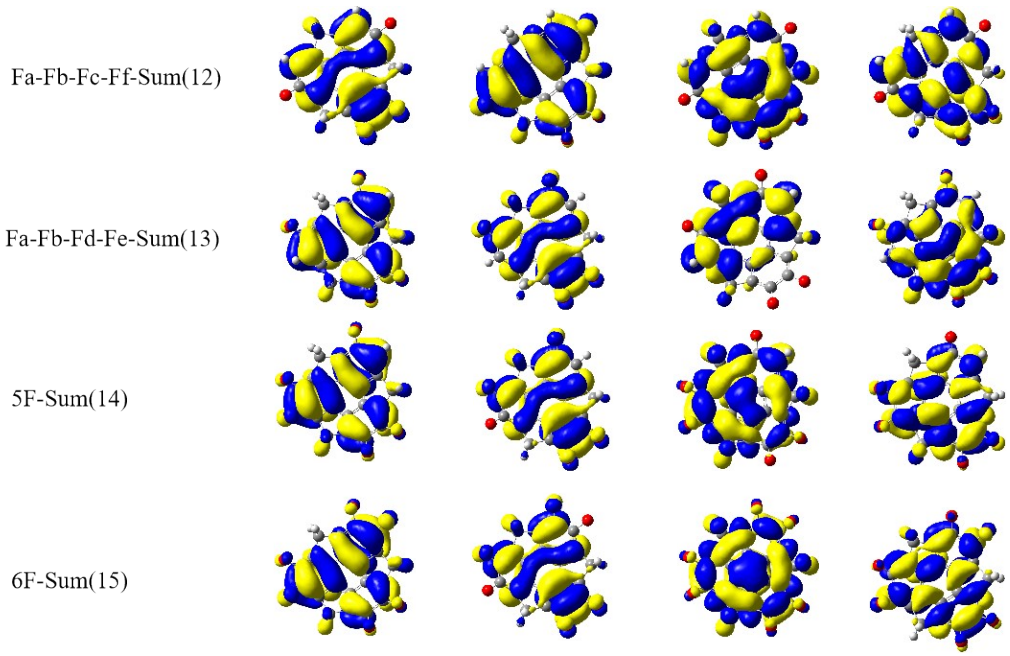


Figure S4. Molecular orbital plots of sumanene and its aromatic-fluorinated derivatives.

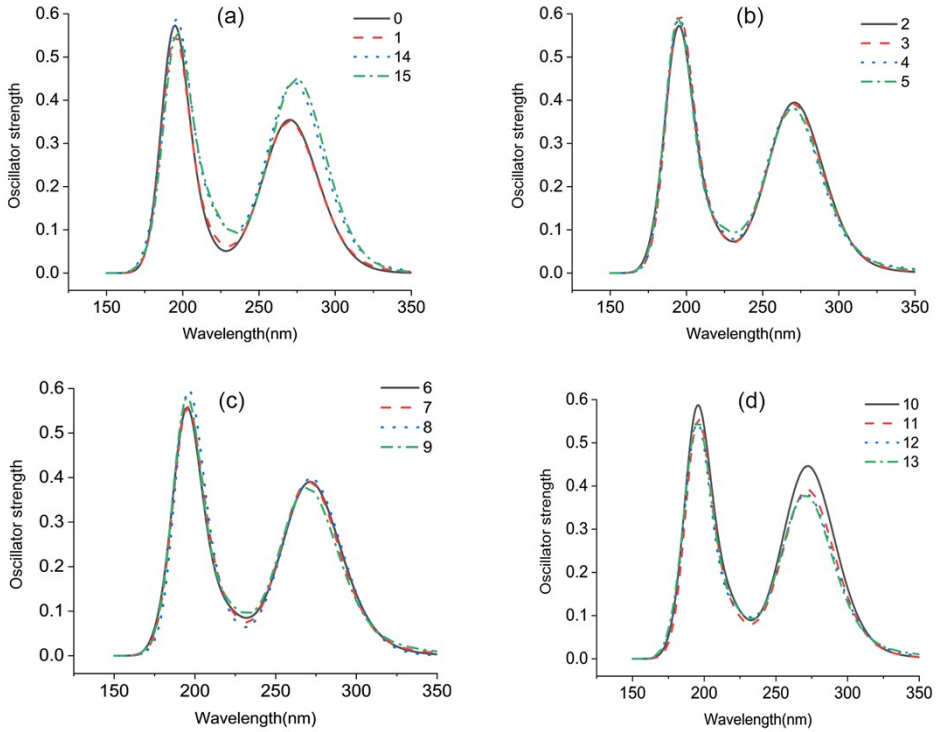


Figure S5. The absorption spectra of sumanene and its aromatic-fluorinated derivatives by calculation.