Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

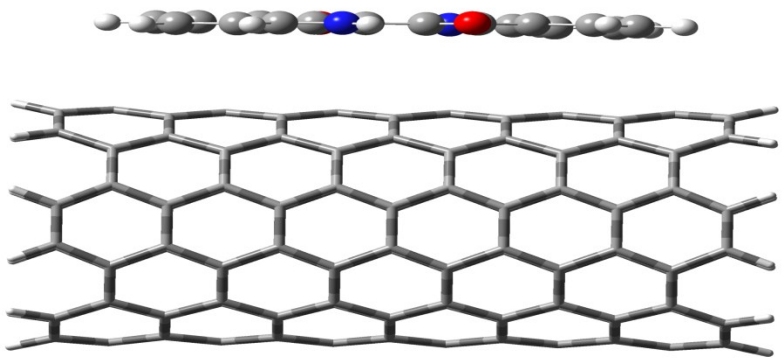


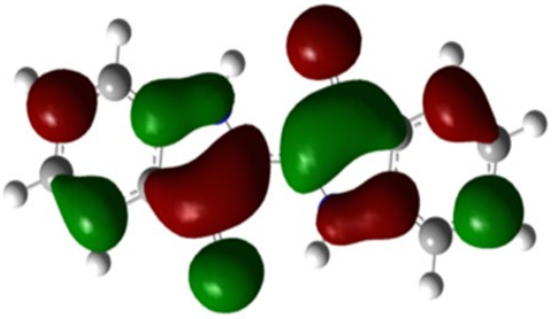
Figure S1. The optimized geometry of the complex in which indigo is aligned parallel to the tube axis

Table S1. Stabilization energy of dyad and triad using different functional at 6-31G** level

Functional	**ΔE_{stab} of dyad (kcal/mol)**	**ΔE_{stab} of triad (kcal/mol)**
B97-D	-28.27	-56.75
B3LYP-GD2	-27.85	-55.94
M062X	-18.36	-37.03
CAM-B3LYP	4.17	8.39
B3LYP	11.85	23.71

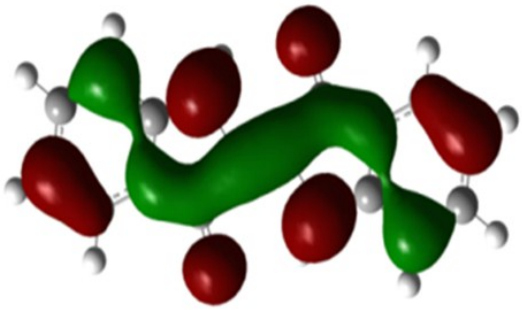
Table S2. The calculated values of absorption wavelengths, corresponding oscillator strengths, prominent molecular orbitals involved and the respective percentage contribution for Indigo, CNT and their complexes. The isodensity plot of molecular orbitals is also shown.

Indigo

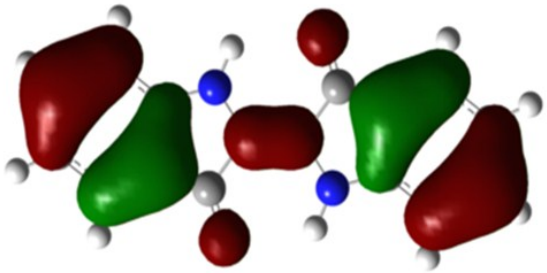


LUMO

λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
614	0.22	HOMO → LUMO	99
384	0.12	HOMO-4 → LUMO	89



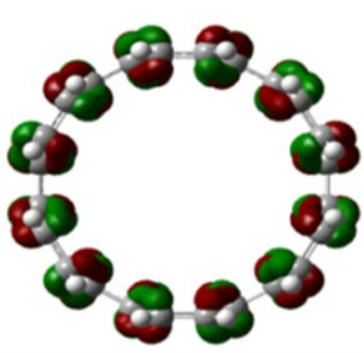
HOMO



HOMO-4

CNT

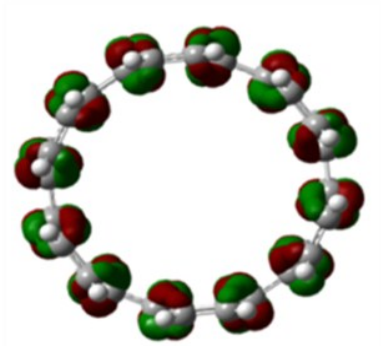
LUMO



LUMO+1

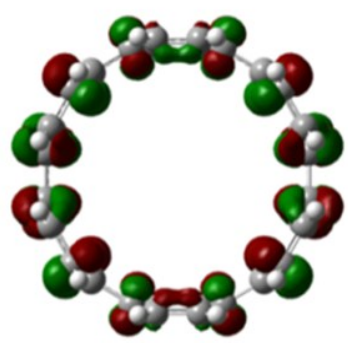
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
874	0.68	HOMO-1 → LUMO	51
		HOMO → LUMO+1	46

HOMO-1



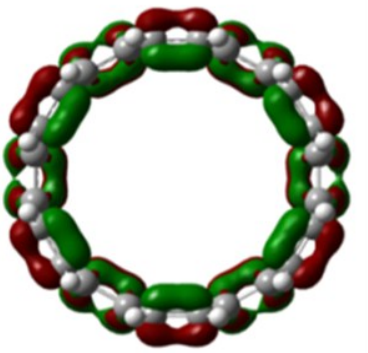
HOMO

LUMO+2



LUMO+3

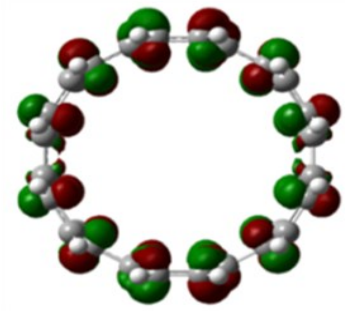
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
548	0.21	HOMO-2 → LUMO+3	37
429	0.07	HOMO-8 → LUMO+2	31



HOMO-8

HOMO-2

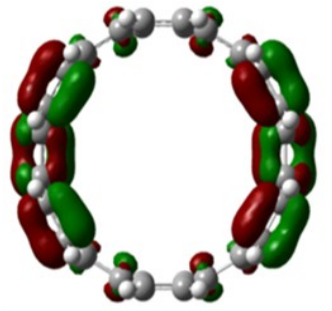
LUMO+14



LUMO+4

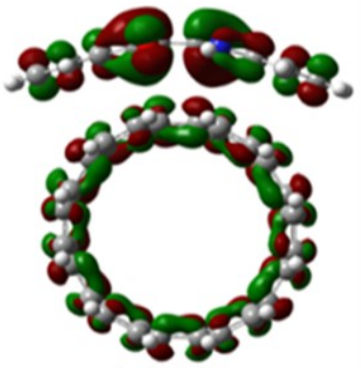
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
429	0.07	HOMO -2 → LUMO+14	36
399	1.17	HOMO-9 → LUMO+4	22

HOMO-2

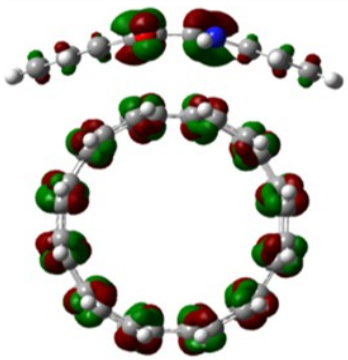


HOMO-9

Dyad

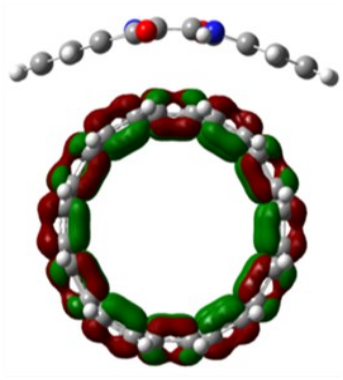


LUMO

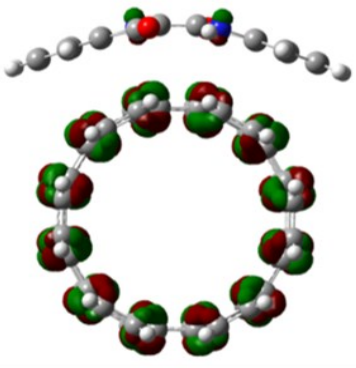


LUMO+2

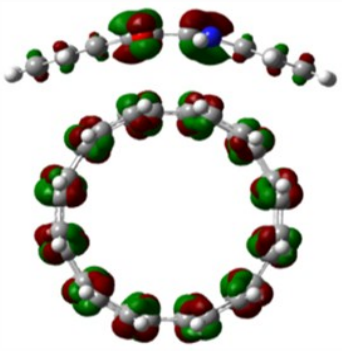
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
884	0.58	HOMO-1 →LUMO	25
		HOMO → LUMO+2	37



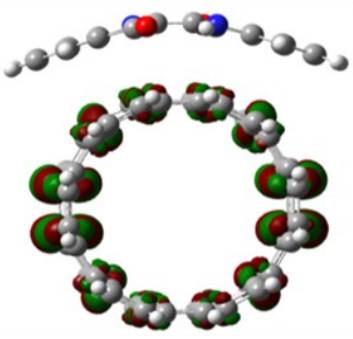
HOMO-1



HOMO

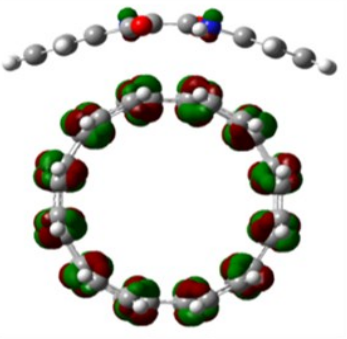


LUMO+2



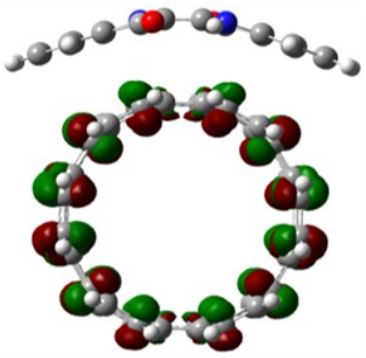
LUMO+18

HOMO-2

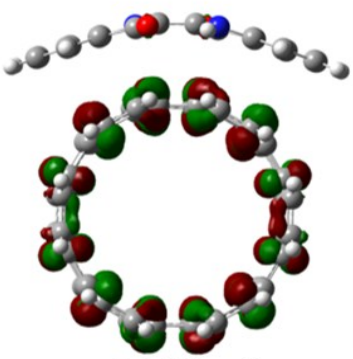


HOMO

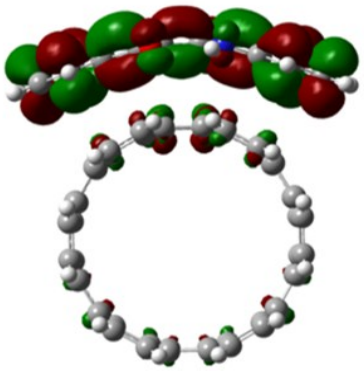
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
805	0.06	HOMO -2 → LUMO+2	69
549	0.11	HOMO → LUMO+18	54



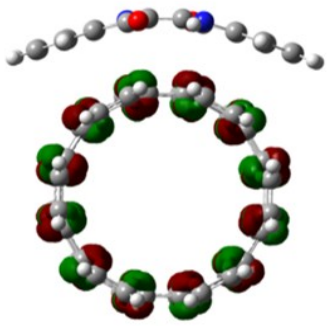
LUMO+4



LUMO+5

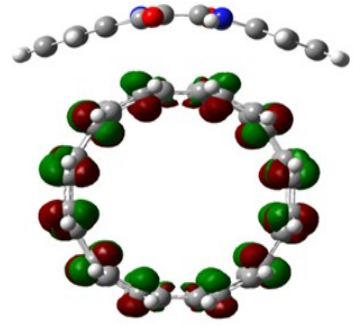


LUMO+19

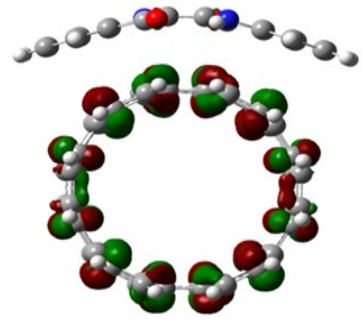


HOMO-3

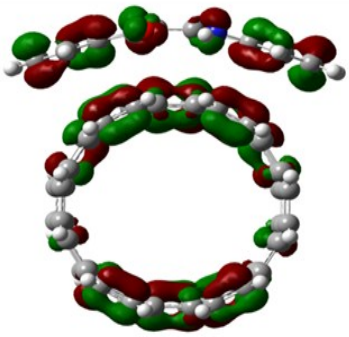
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
549	0.19	HOMO-3 →LUMO+4	35
539	0.10	HOMO -3 → LUMO+5	31
401	0.07	HOMO -3 → LUMO+19	62



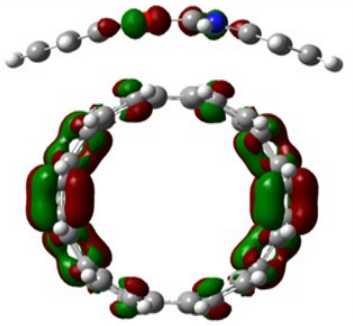
LUMO+4



LUMO+5



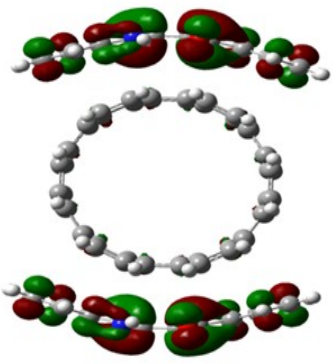
HOMO-13



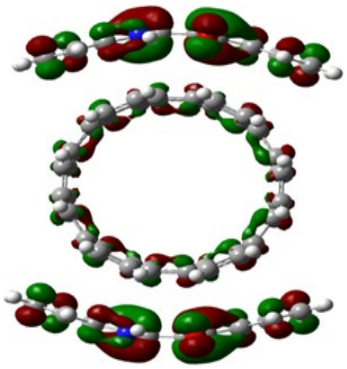
HOMO-11

λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
399.7	0.83	HOMO-13 →LUMO+4	17
		HOMO-11 →LUMO+5	19

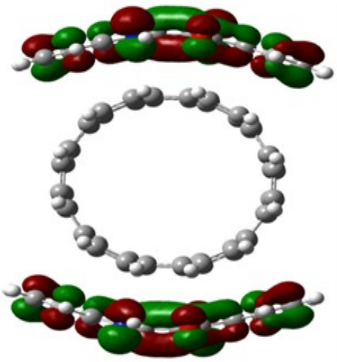
Triad



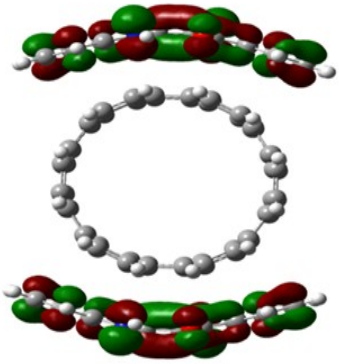
LUMO+1



LUMO+2

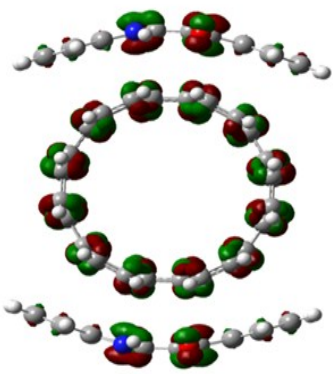


HOMO-3

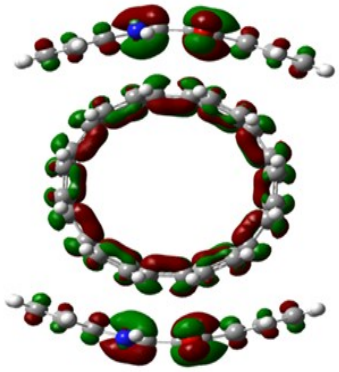


HOMO-2

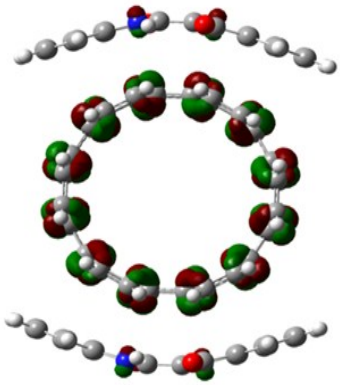
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
897	0.08	HOMO-3 → LUMO+1	30
		HOMO -2 → LUMO+2	50



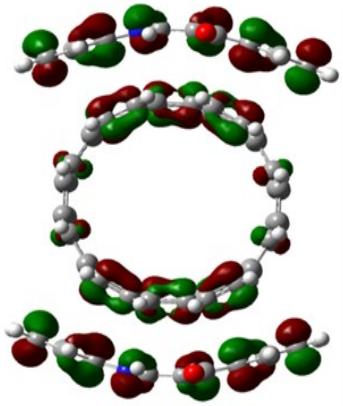
LUMO+3



LUMO

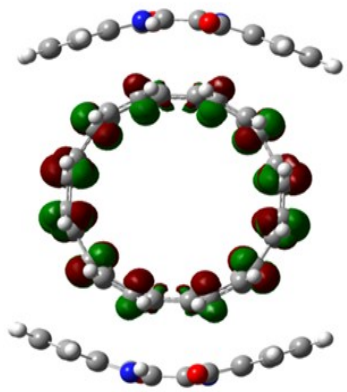


HOMO

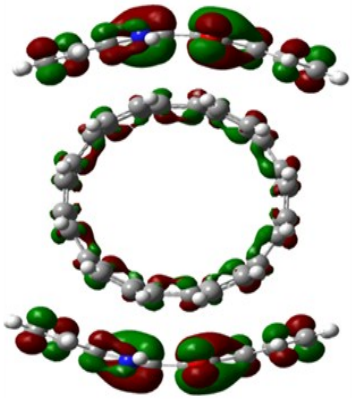


HOMO-11

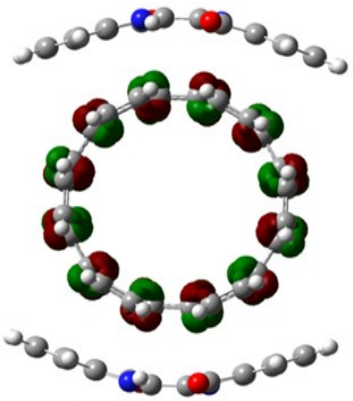
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
887	0.47	HOMO → LUMO+3	30
585	0.05	HOMO-11 → LUMO	74



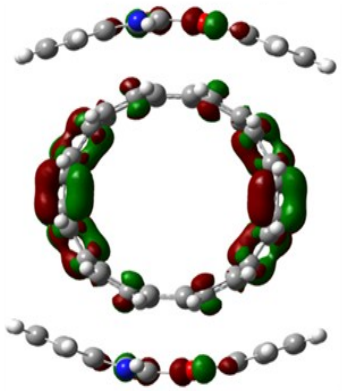
LUMO+5



LUMO+2

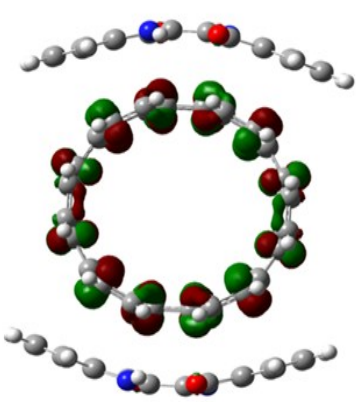


HOMO-4

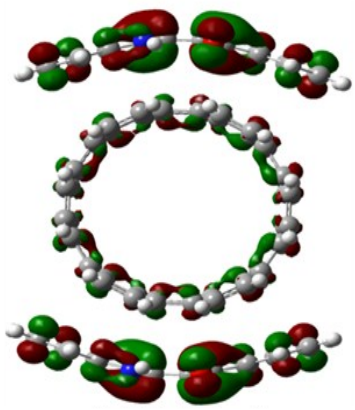


HOMO-13

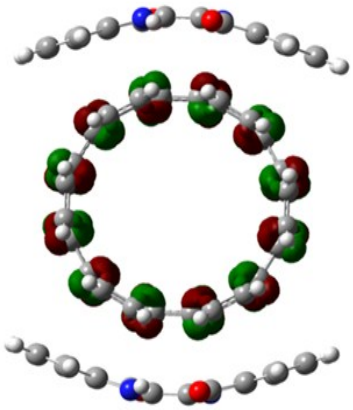
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
551	0.15	HOMO-4 →LUMO+5	30
549	0.12	HOMO-13 →LUMO+2	74



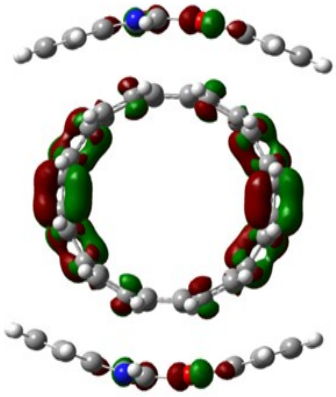
LUMO+6



LUMO+2

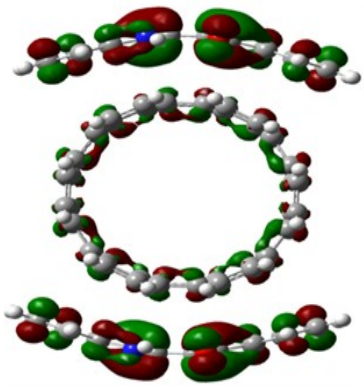


HOMO-4

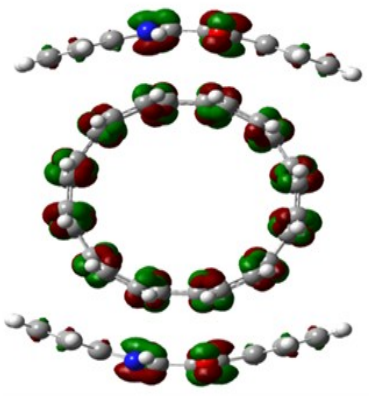


HOMO-13

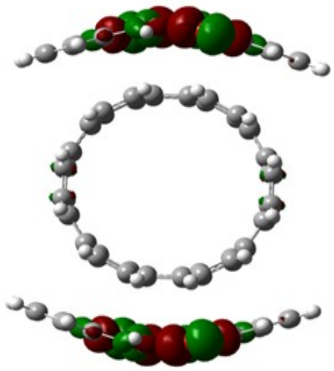
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
542	0.10	HOMO-4 → LUMO+6	42
539	0.07	HOMO-13 →LUMO+2	32



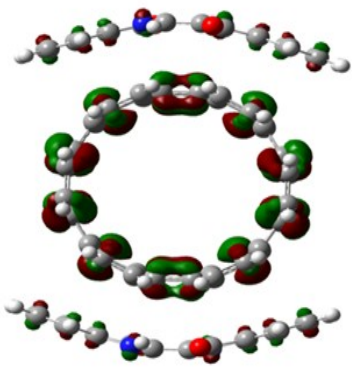
LUMO+2



LUMO+3

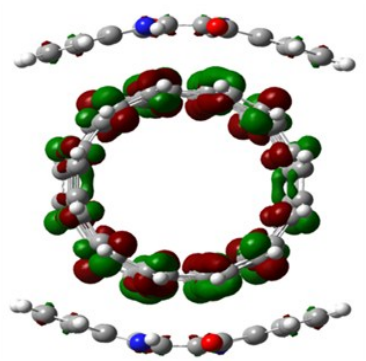


HOMO-14



HOMO-9

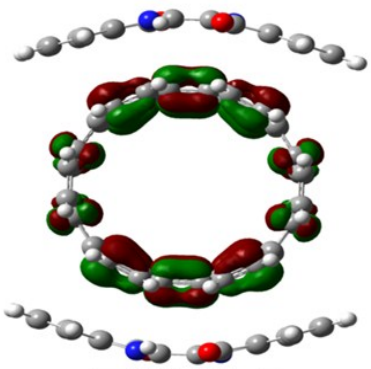
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
536	0.06	HOMO-14 → LUMO+2	30
		HOMO-9 →LUMO+3	44



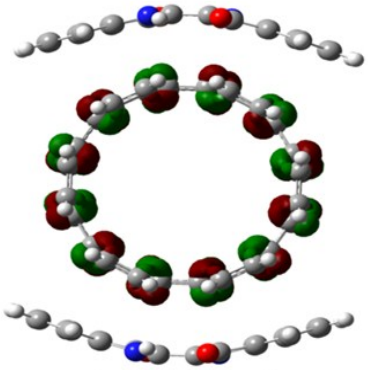
LUMO+14

LUMO+20

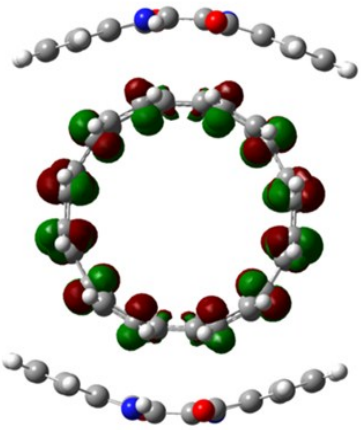
λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
428	0.05	HOMO-5 → LUMO+14	48
404	0.08	HOMO-4 →LUMO+20	56



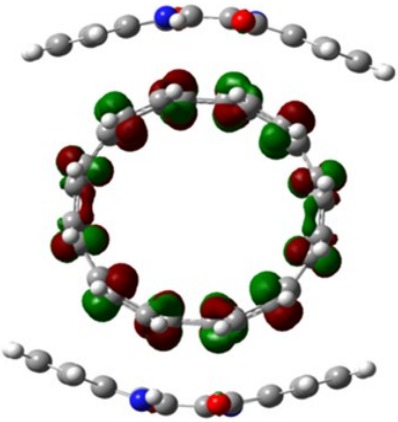
HOMO-5



HOMO-4

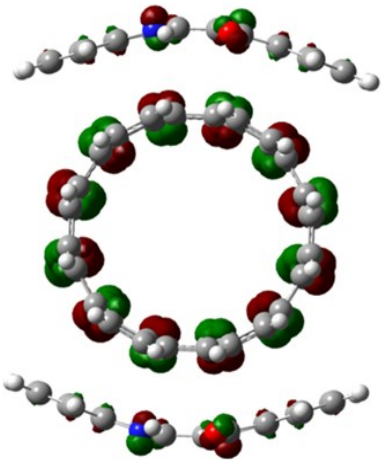


LUMO+5

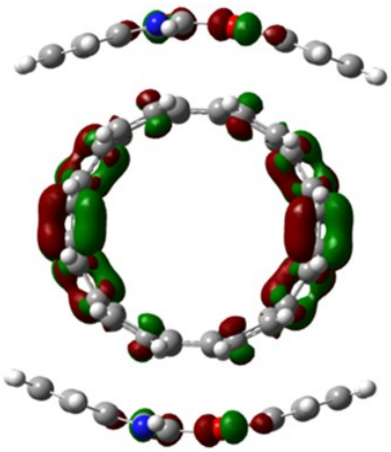


LUMO+6

λ_{max} (nm)	Oscillator Strength	Molecular orbitals involved	Contribution (in %)
400.4	0.42	HOMO-17 → LUMO+5	12
		HOMO-13 → LUMO+6	16



HOMO-17



HOMO-13