Supplementary Information

Photophysical and Photochemical Properties and Aggregation Behavior of Phthalocyanine and Naphthalocyanine Derivatives

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Table S1. Electronic absorption spectra data as obtained with TD-DFT in DMSO (IEFPCM)

	λ^a / nm	Oscillator strength	Molecular orbital (MO)
ZnPc	674	0.4641	HOMO → LUMO; HOMO → LUMO+1
	425	0.0096	HOMO-1 → LUMO; HOMO-1 → LUMO+1
1	687	0.5369	HOMO → LUMO; HOMO → LUMO+1
	437	0.0269	HOMO-1 → LUMO; HOMO-1 → LUMO+1
ZnNc	770	0.6578	HOMO → LUMO; HOMO → LUMO+1
	489	0.0167	HOMO → LUMO+3; HOMO → LUMO+4
	465	0.2673	HOMO-1 → LUMO; HOMO-1 → LUMO+1
2	789	0.7024	HOMO → LUMO; HOMO → LUMO+1
	489	0.0092	HOMO → LUMO+4
	485	0.0060	HOMO → LUMO+5
	477	0.0422	HOMO-2 → LUMO; HOMO-1 → LUMO
	471	0.2010	HOMO-1 → LUMO+1
	470	0.2334	HOMO-1 → LUMO

[a]Wavelength fitted to experimental data by a factor of 16% for ZnPc and **1** and 10% ZnNc (calculated from the difference between calculated and experimental Q-band). Fit parameters are different because DFT predicts better gap energy as larger is the conjugated system.

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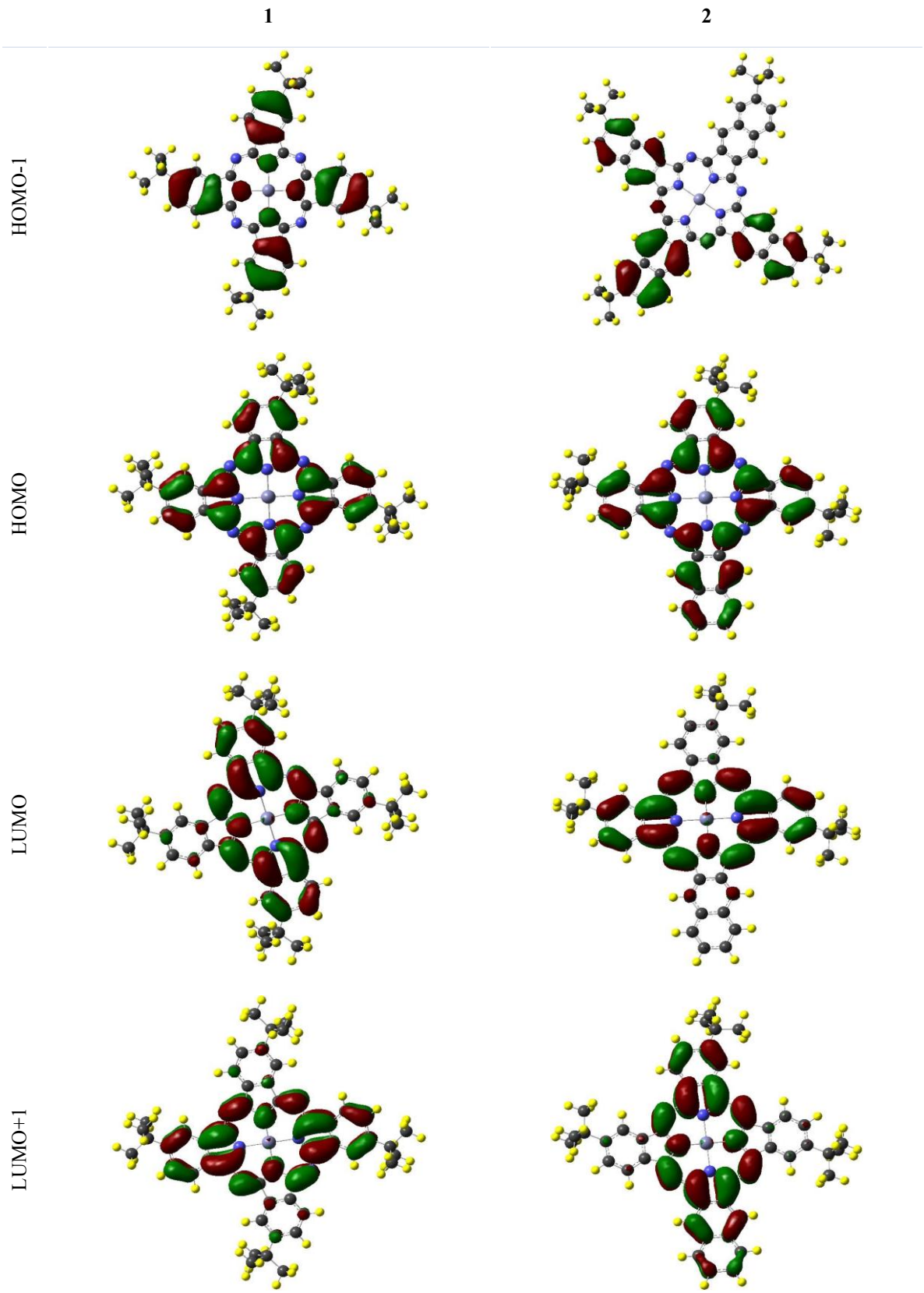
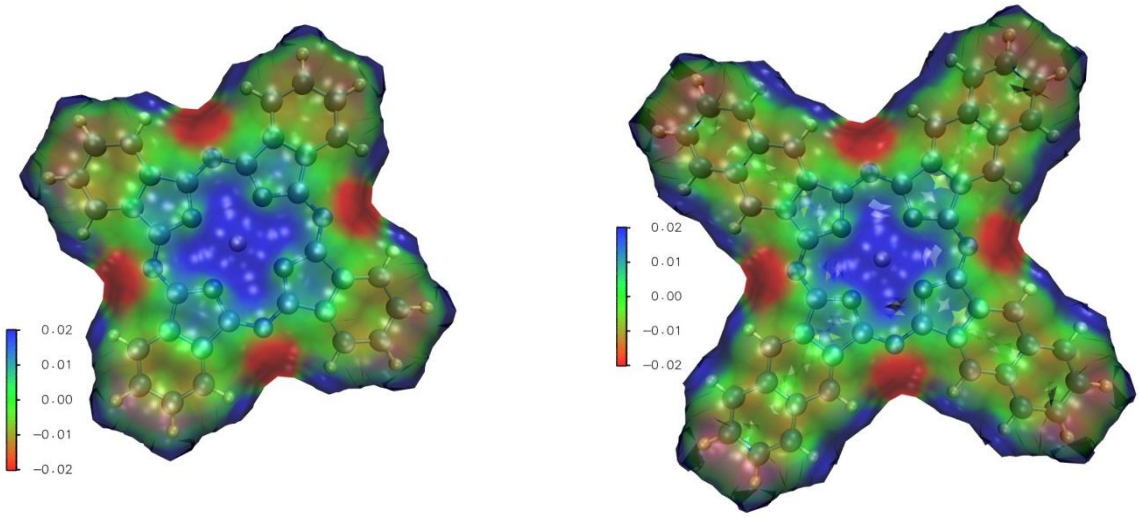


Figure S1. Frontier molecular orbitals for **1** and **2**.

Table S2. Electronic absorption spectra data (wavelength (λ) and oscillator strength (*f*)) for Q-band of each compound as obtained with TD-DFT using different solvents (simulated with IEFPCM, values in parenthesis correspond to the dielectric constant)

	Toluene (2.4)		DCM (8.9)		DMF (37.2)		DMSO (46.8)		$CHCl_3$ (47.1)	
	λ^a / nm	*f*	λ^a / nm	*f*	λ^a / nm	*f*	λ^a / nm	*f*	λ^a / nm	*f*
ZnPc	674.0346	0.4649	674.0346	0.4649	674.0855	0.4638	674.0776	0.4640	674.0346	0.4649
1	686.6262	0.5378	686.6262	0.5378	686.5937	0.5367	686.6018	0.5369	686.6262	0.5378
ZnNc	770.2865	0.6584	770.2865	0.6584	770.1463	0.6577	770.1733	0.6578	770.2865	0.6584
2	789.5039	0.7027	789.5039	0.7027	789.1641	0.7023	789.2320	0.7024	789.5039	0.7027

[a]Wavelength fitted to experimental data by a factor of 16% for ZnPc and **1** and 10% ZnNc (calculated from the difference between calculated and experimental Q-band). Fit parameters are different because DFT predicts better gap energy as larger is the conjugated system. DCM: dichloromethane; DMF: dimethylformamide; DMSO: dimethyl sulfoxide.



(a) (b)

Figure S2. Electrostatic potential surface mapped obtained for (a) ZnPc and (b) ZnNc (values in atoms units).

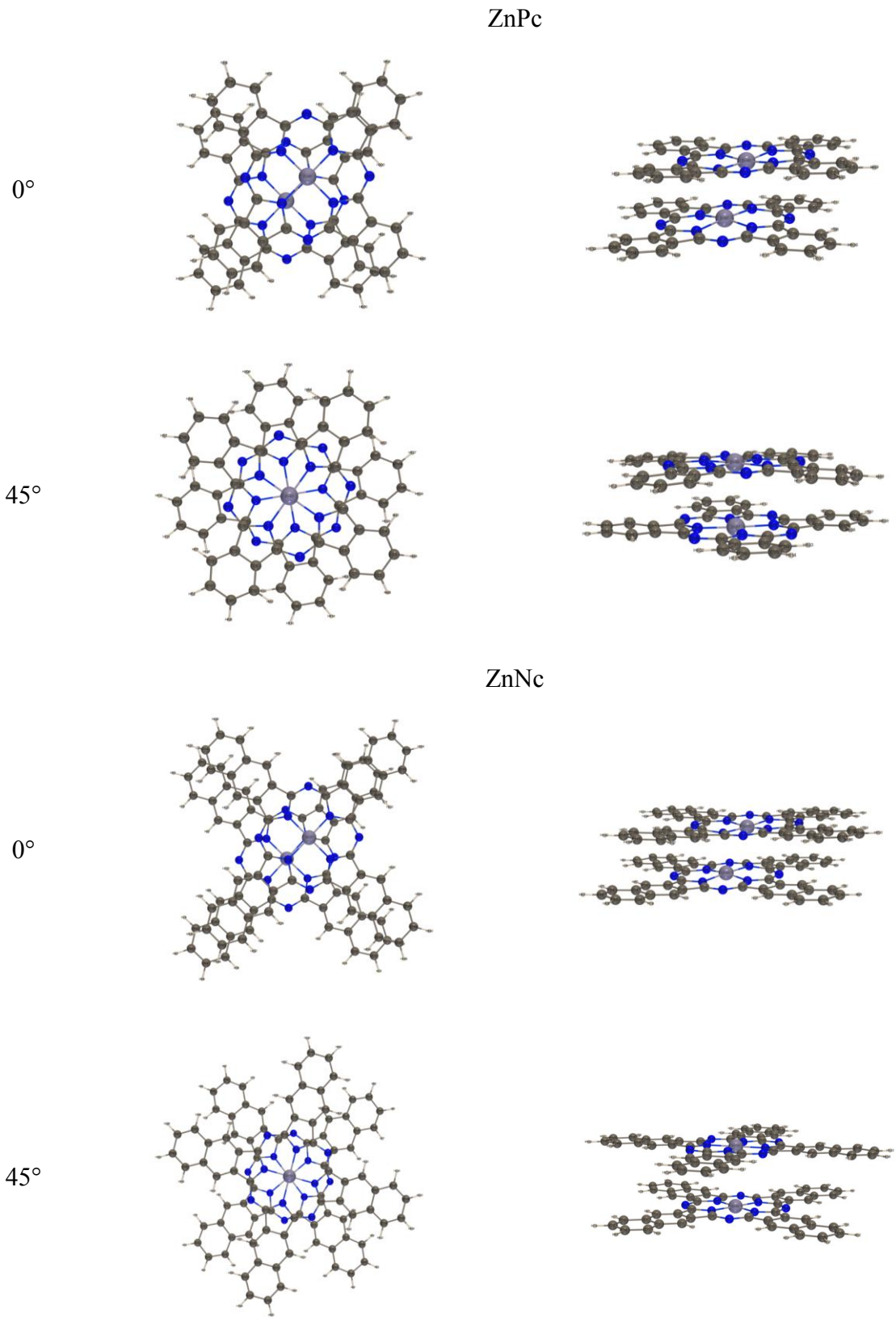


Figure S3. Aggregate conformations found for ZnPc and ZnNc, top view (left) and side view (right).

Table S3. Electronic absorption spectra data as obtained with TD-DFT calculations for dimeric species (in DMSO, as simulated with IEFPCM)

	λ^a / nm	Oscillator strength	Molecular orbital (MO)
ZnPc 0°	670	0.4445	HOMO-1 → LUMO+2; HOMO → LUMO+1
	668	0.4206	HOMO-1 → LUMO; HOMO → LUMO+3
	636	0.0402	HOMO-3 → LUMO+1
ZnPc 45°	660	0.4358	HOMO-1 → LUMO+1; HOMO-1 → LUMO
	657	0.0156	HOMO-2 → LUMO
ZnNc 0°	758	0.5610	HOMO → LUMO+3; HOMO-1 → LUMO
	756	0.6065	HOMO-1 → LUMO+1; HOMO → LUMO+1
	686	0.2015	HOMO-2 → LUMO
ZnNc 45°	744	0.8628	HOMO-1 → LUMO; HOMO-1 → LUMO+1

[a]Wavelength fitted to experimental data by a factor of 16% for ZnPc and **1** and 10% ZnNc (calculated from the difference between calculated and experimental Q-band). Fit parameters are different because DFT predicts better gap energy as larger is the conjugated system.

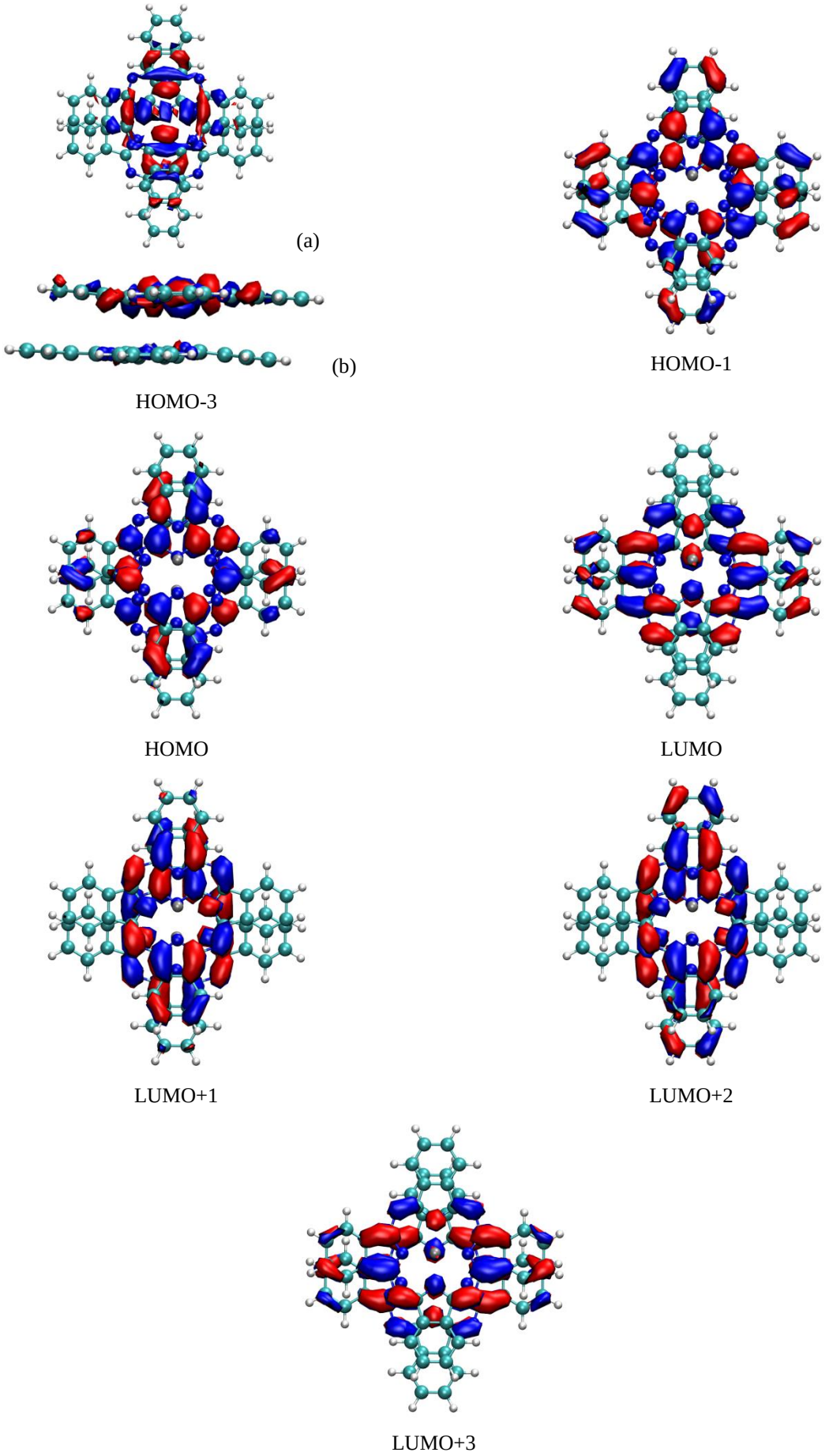


Figure S4. Molecular orbitals ((a) top view, (b) side view) involved in the main transitions of dimer 0° of ZnPc.

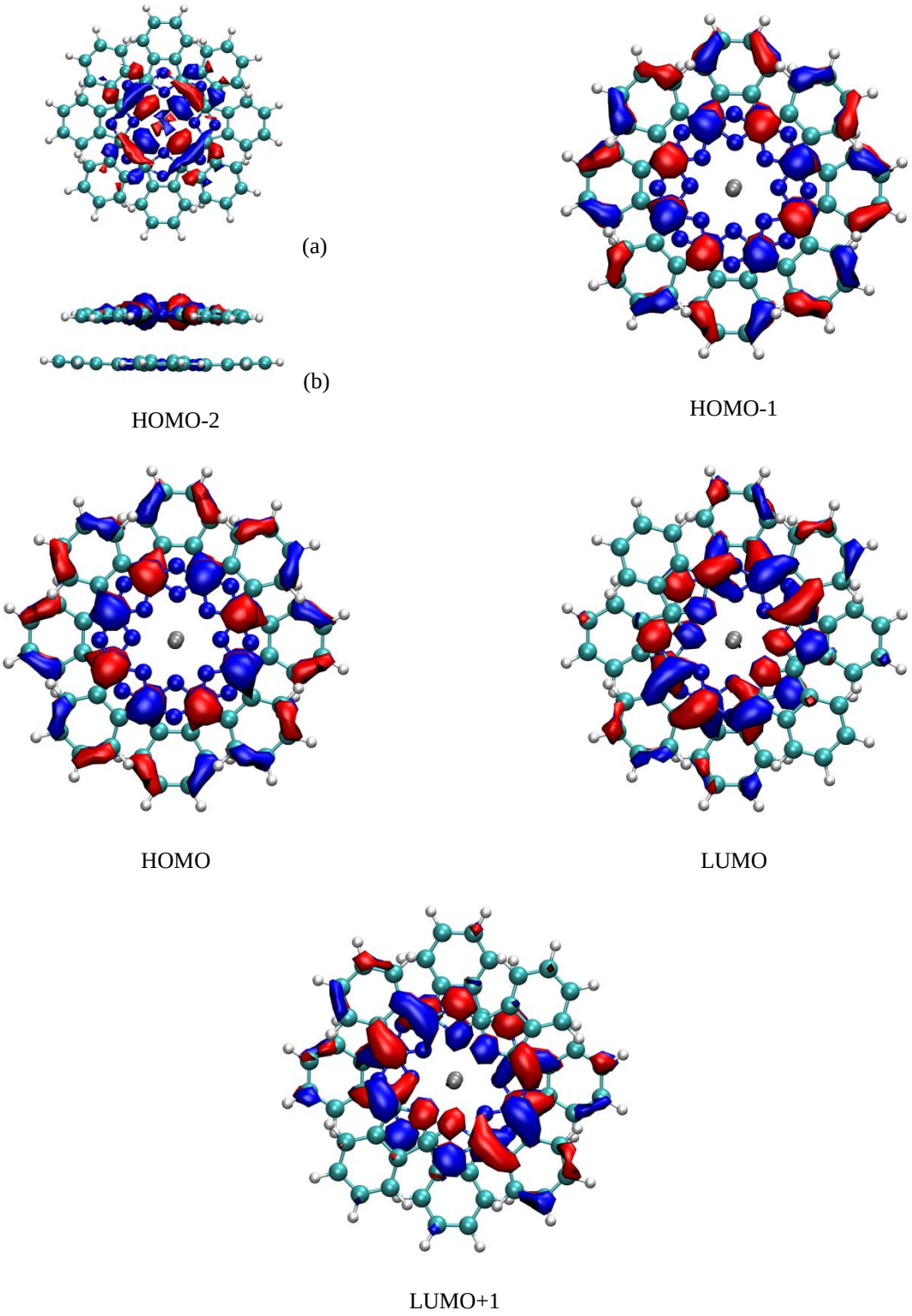
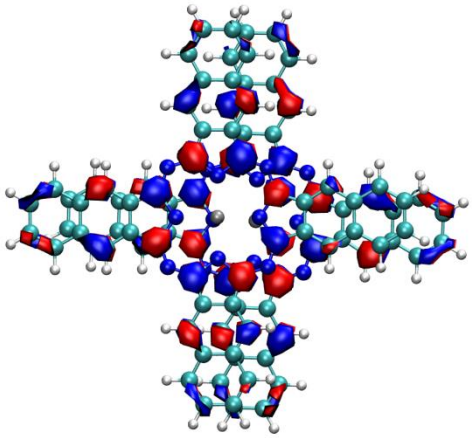
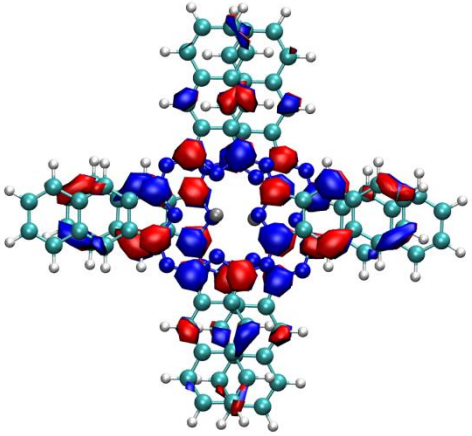


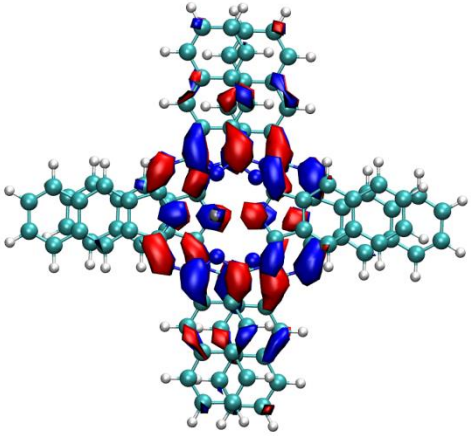
Figure S5. Molecular orbitals ((a) top view, (b) side view) involved in the main transitions of dimer 45° of ZnPc.



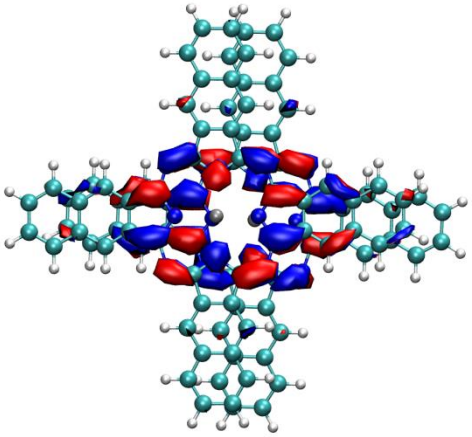
HOMO-1



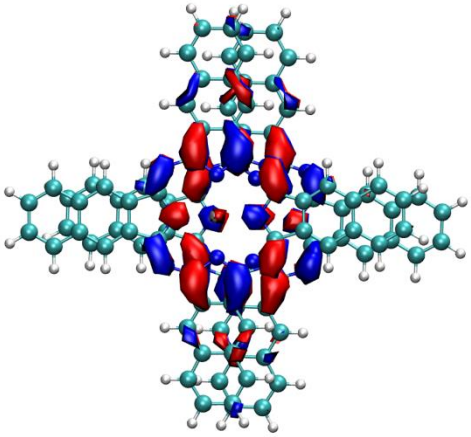
HOMO



LUMO

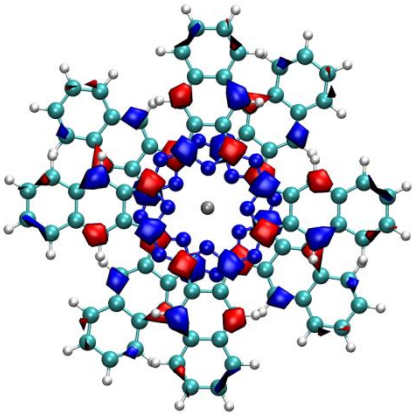


LUMO+1

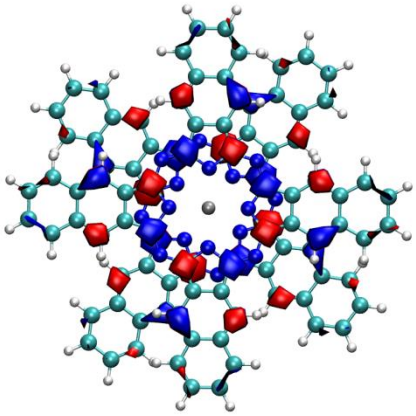


LUMO+3

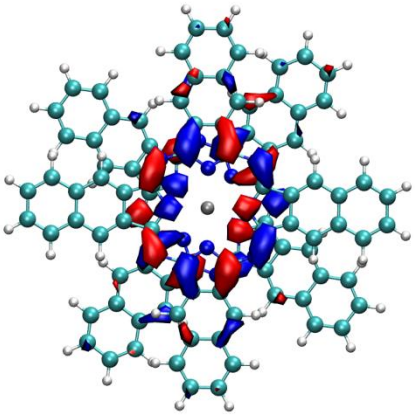
Figure S6. Molecular orbitals involved in the main transitions of dimer 0° of ZnNc.



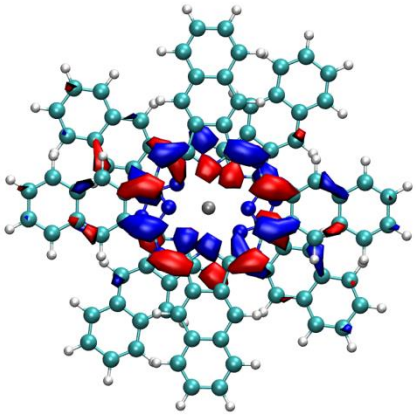
HOMO-1



HOMO



LUMO



LUMO+1

Figure S7. Molecular orbitals involved in the main transitions of dimer 45^{o} of ZnPc.