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

Effects of Aggregation on the Structures and Excited-State Absorption for Zinc Phthalocyanine(Supporting Information)

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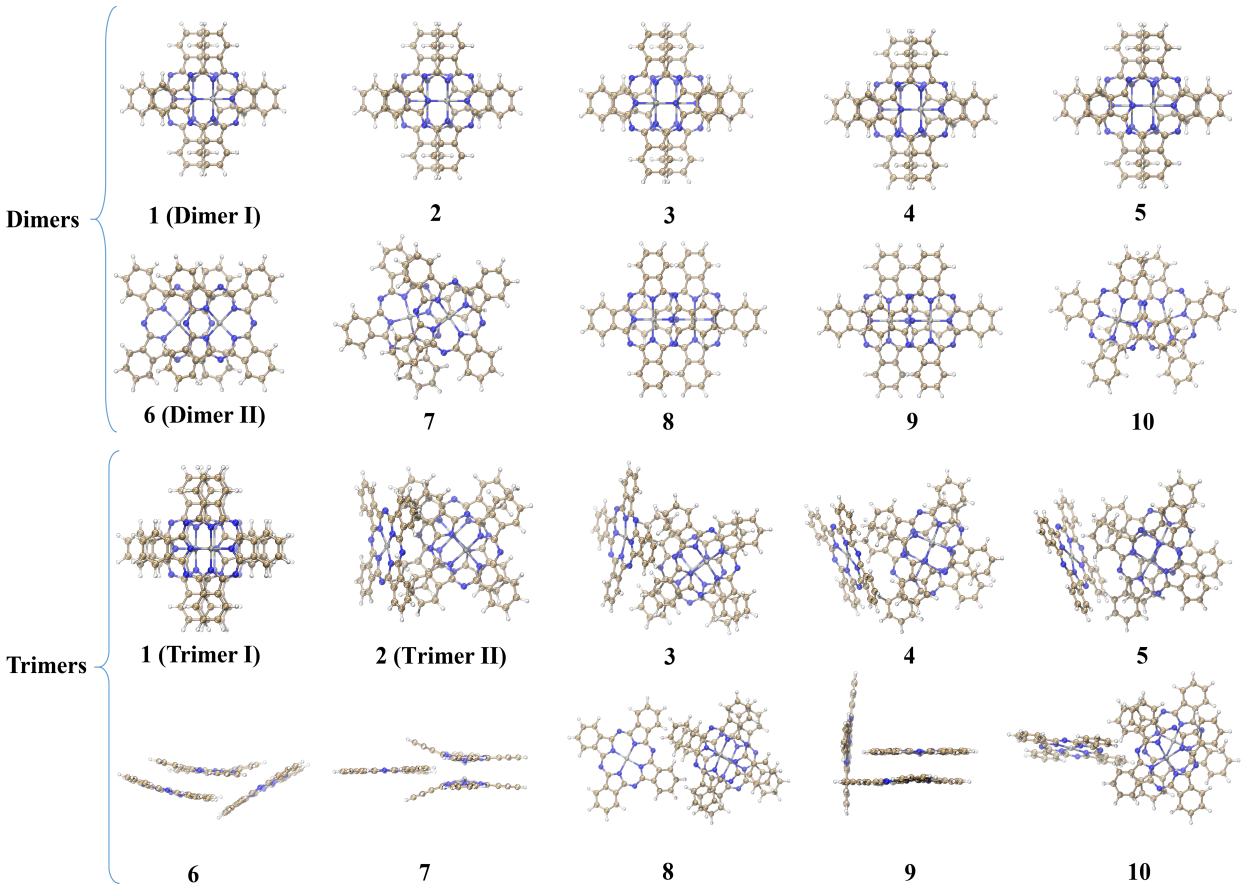


FIG. S1: Ten conformations for the ZnPc dimers and trimers, which are optimized based on DFT with dispersion-corrected B3LYP functional and 6-31G(d,p) basis set applied.

TABLE S1: The energies of the choosing 10 conformations for the ZnPc dimers and trimers. Energies are in atomic unit.

Dimers	Energy	Trimers	Energy
1(Dimer I)	-6893.2089253	1(Trimer I)	-10339.8586720
2	-6893.2089253	2(Trimer II)	-10339.8101839
3	-6893.2089253	3	-10339.8074335
4	-6893.2089252	4	-10339.8043153
5	-6893.2089252	5	-10339.8032960
6(Dimer II)	-6893.2003725	6	-10339.8013140
7	-6893.1990331	7	-10339.7930560
8	-6893.1971760	8	-10339.7914220
9	-6893.1971759	9	-10339.7903561
10	-6893.1923945	10	-10339.7875755

TABLE S2: The binding energies (kcal/mol) of the ZnPc dimers and trimers estimated under the B3LYP-D3(BJ) functional and various basis sets.

Systems	6-31G(d,p)	6-311G(d,p)	def-TZVP
Dimer I	-45.62	-46.18	-48.88
Dimer II	-44.25	-45.94	-46.89
Trimer I	-86.78	-89.86	-91.95
Trimer II	-67.49	-68.29	-70.50

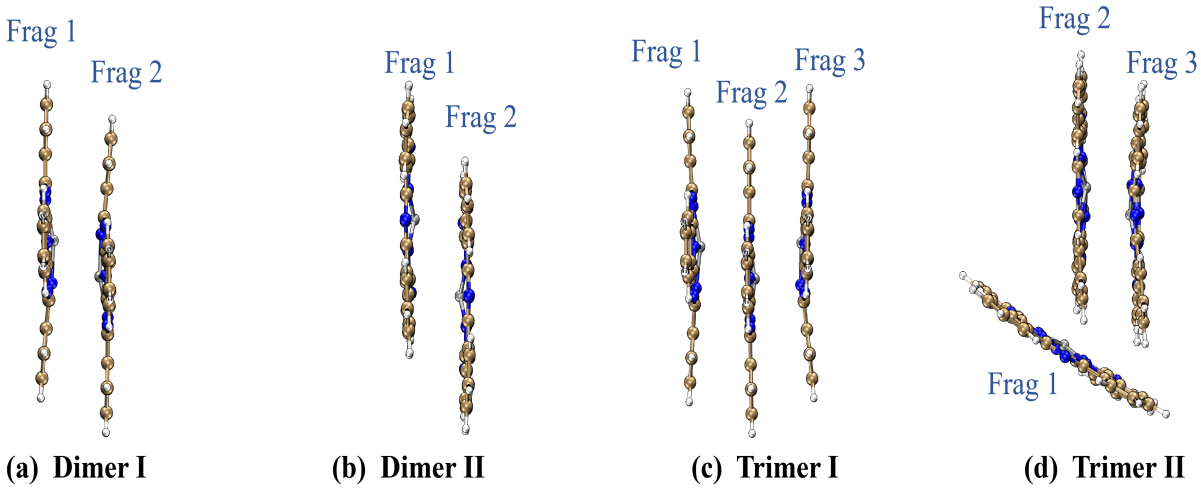


FIG. S2: Fragment definitions in the ZnPc dimers and ZnPc trimers.

TABLE S3: The decomposition of the interaction energy for the ZnPc dimers and Trimers based on the EDA-FF method. All values are given in kJ/mol.

Systems	Fragment	E_{ele}	E_{rep}	E_{disp}	E_{total}
Dimer I	1-2	-8.71	207.89	-360.91	-161.73
Dimer II	1-2	-23.85	173.58	-307.71	-157.98
Trimer I	1-2	4.68	207.43	-361.12	-149.01
	1-3	2.70	0.48	-16.87	-13.98
	2-3	0.56	205.04	-357.87	-152.27
Trimer II	1-2	-3.29	68.57	-98.17	-32.90
	1-3	-3.61	26.00	-61.50	-39.10
	2-3	-8.33	207.00	-360.82	-161.45

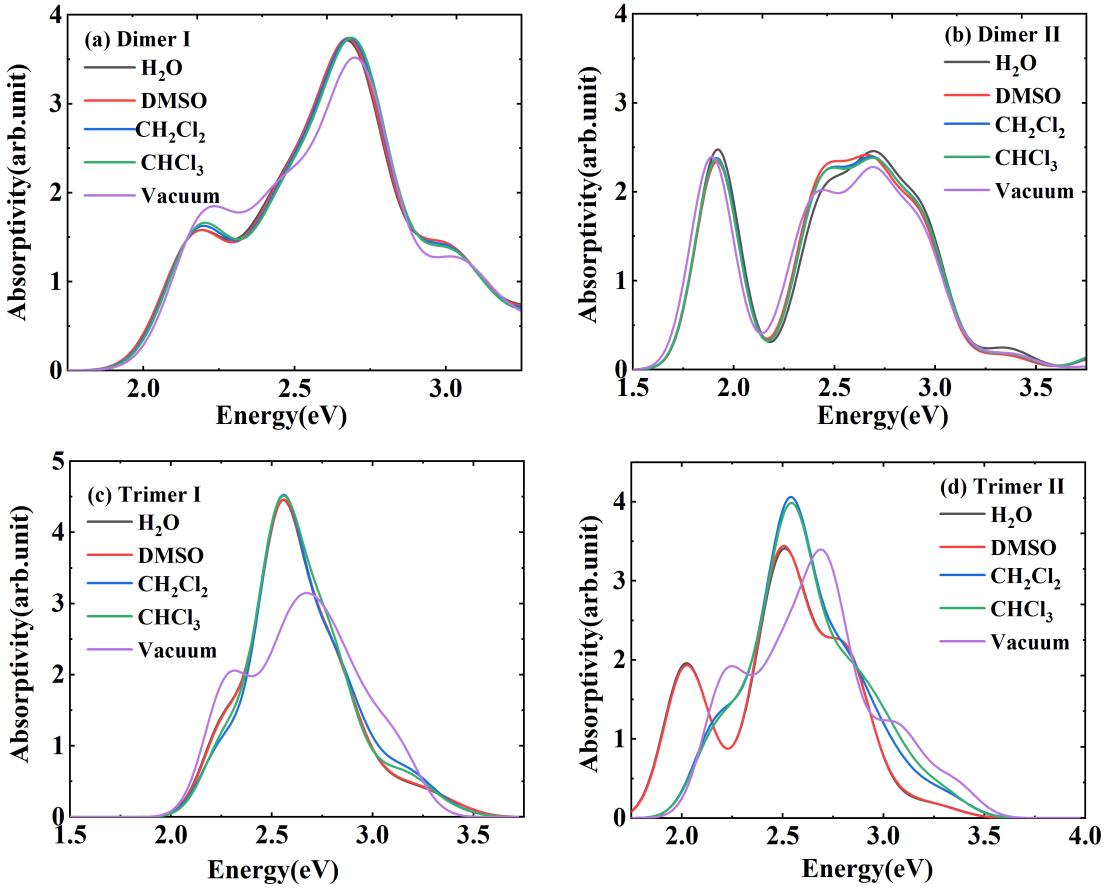
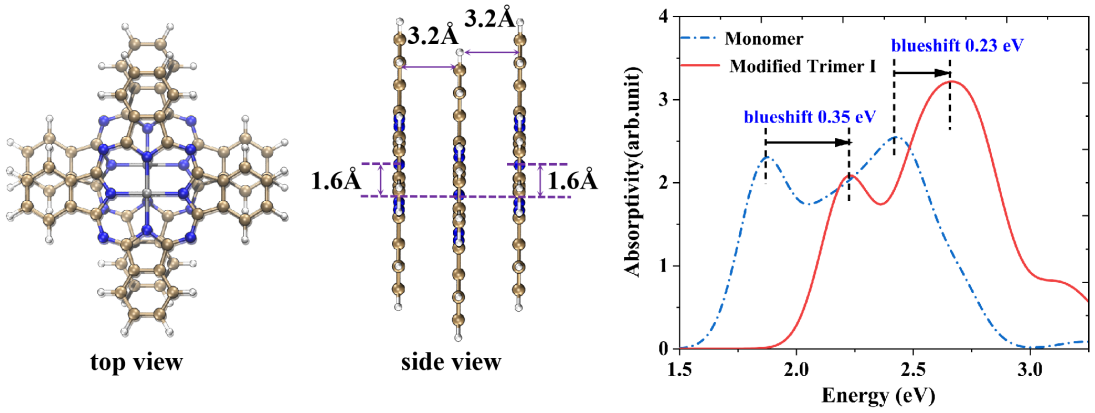


FIG. S3: Comparisions of excited states absorption of ZnPc dimers and ZnPc trimers in various solvents and vacuum.



(a) Structure of Modified Trimer I (b) ESA

FIG. S4: Geometric structure of modified Trimer I and the corresponding ESA.

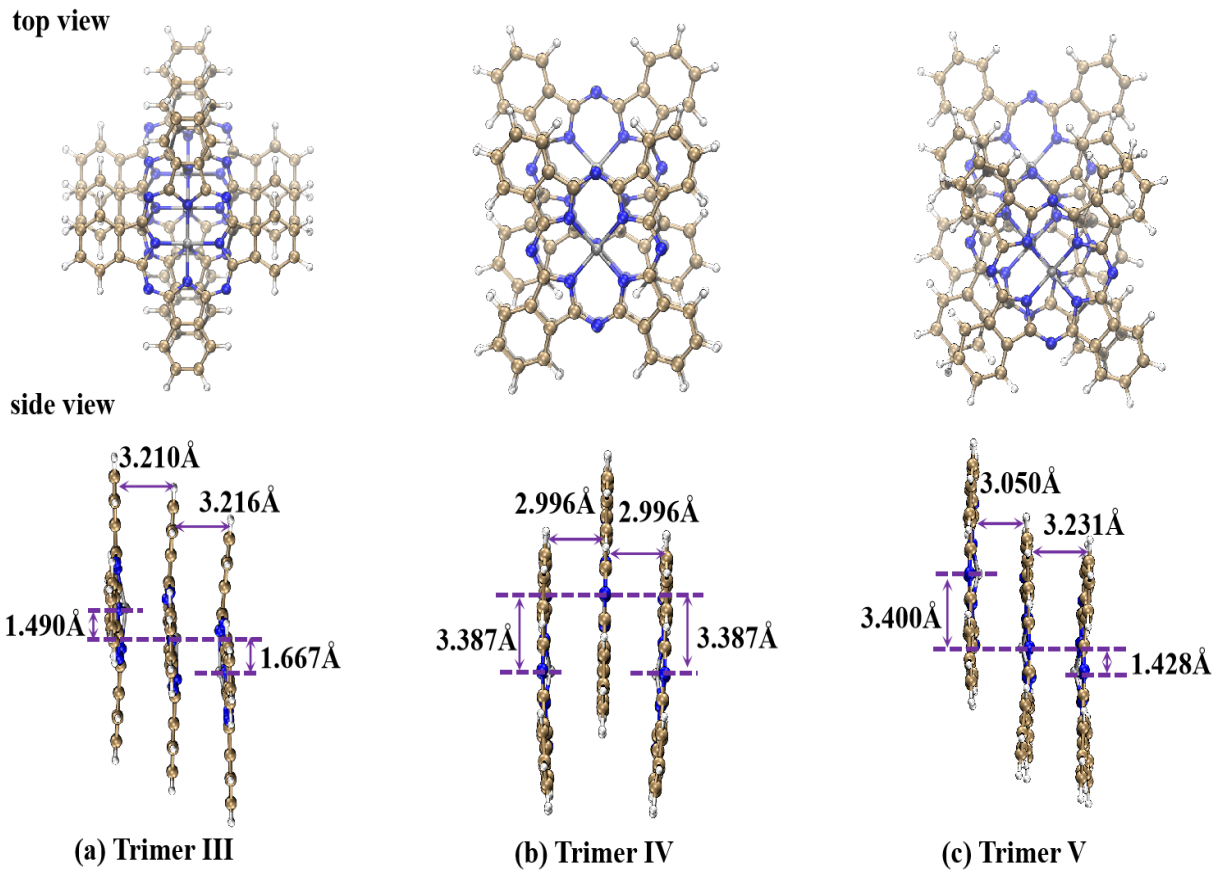


FIG. S5: Geometries of ZnPc Trimer III, Trimer IV and Trimer V optimized at the B3LYP-D3(BJ)/6-31G(d,p) level in the ground state.

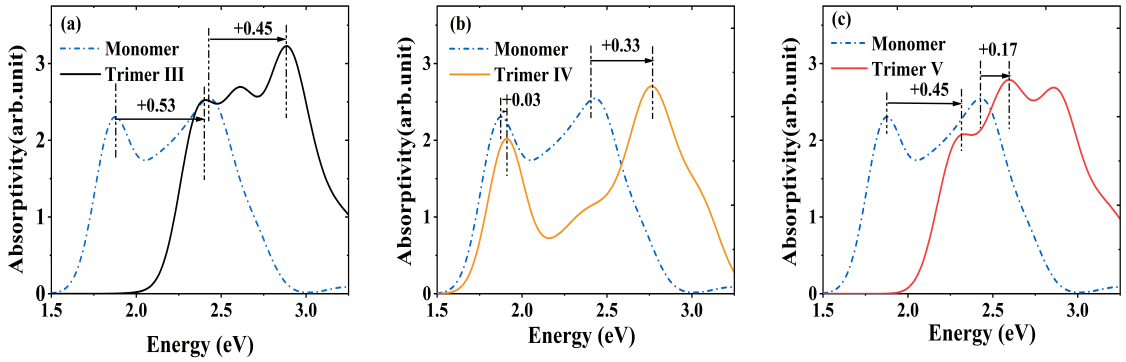


FIG. S6: Comparisons of the ESA in ZnPc Monomer, Trimer III, Trimer IV and Trimer V.

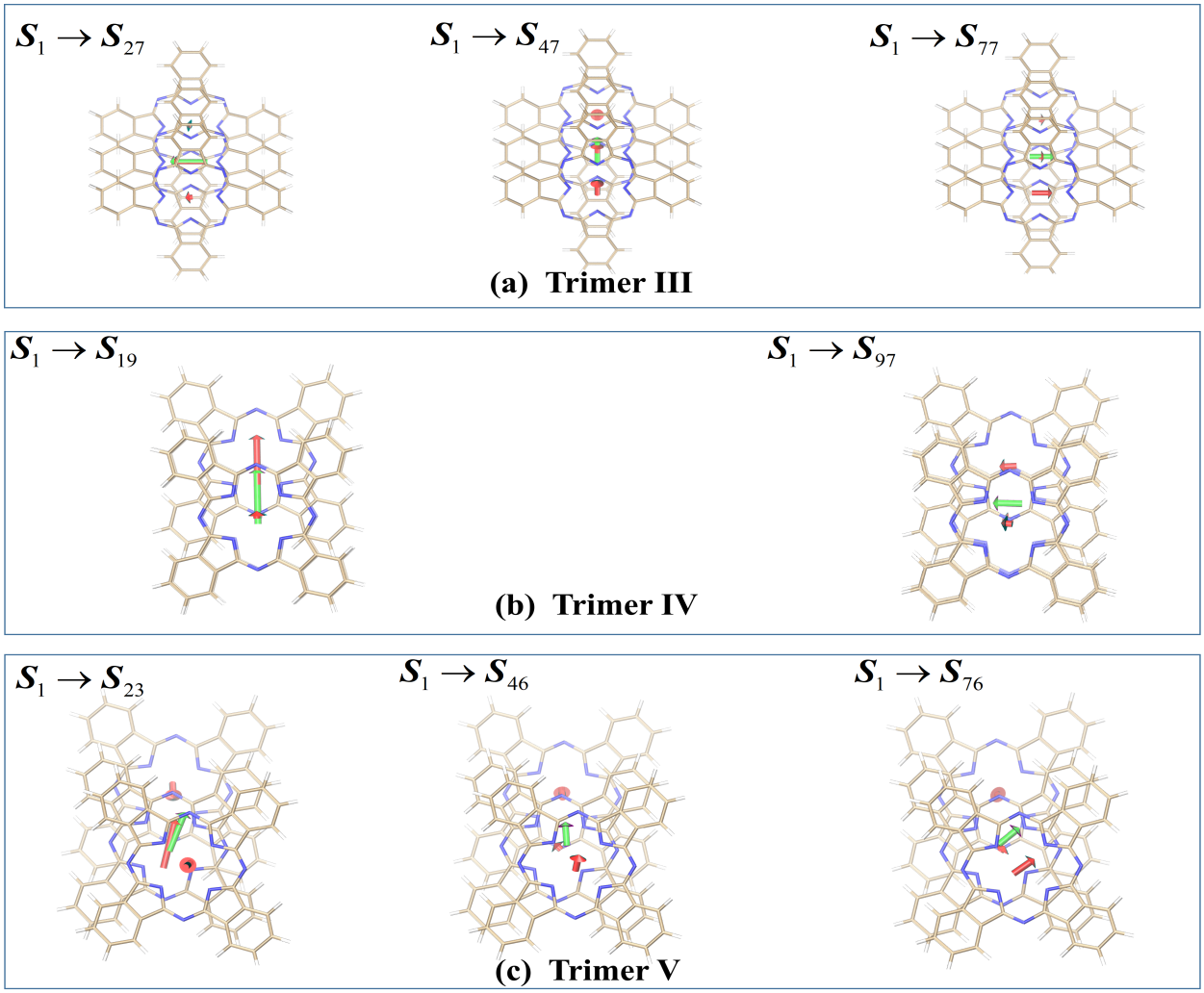


FIG. S7: Transition dipole moment vector contributed by different ZnPc monomers in Trimer III, Trimer IV and Trimer V. The red arrows represent the contribution of each monomer, and the green arrows represent the total transition dipole moment vector of the entire system. The length of the cylindrical part of the arrow corresponds to the size of the transition dipole moment contributed by the fragment, and the direction of the arrow indicates the direction of the transition dipole moment vector.

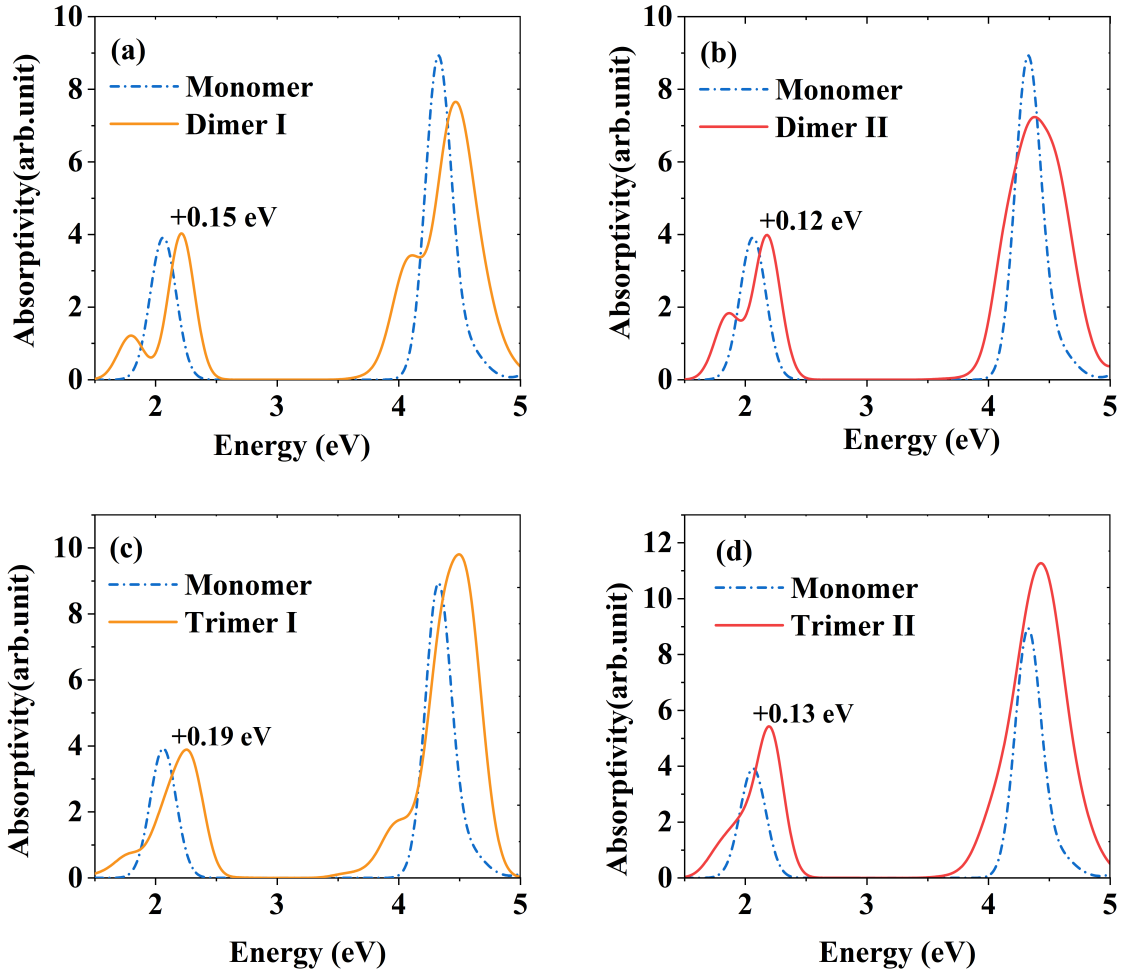


FIG. S8: Comparisons of the GSA in ZnPc monomer, dimers and trimers.

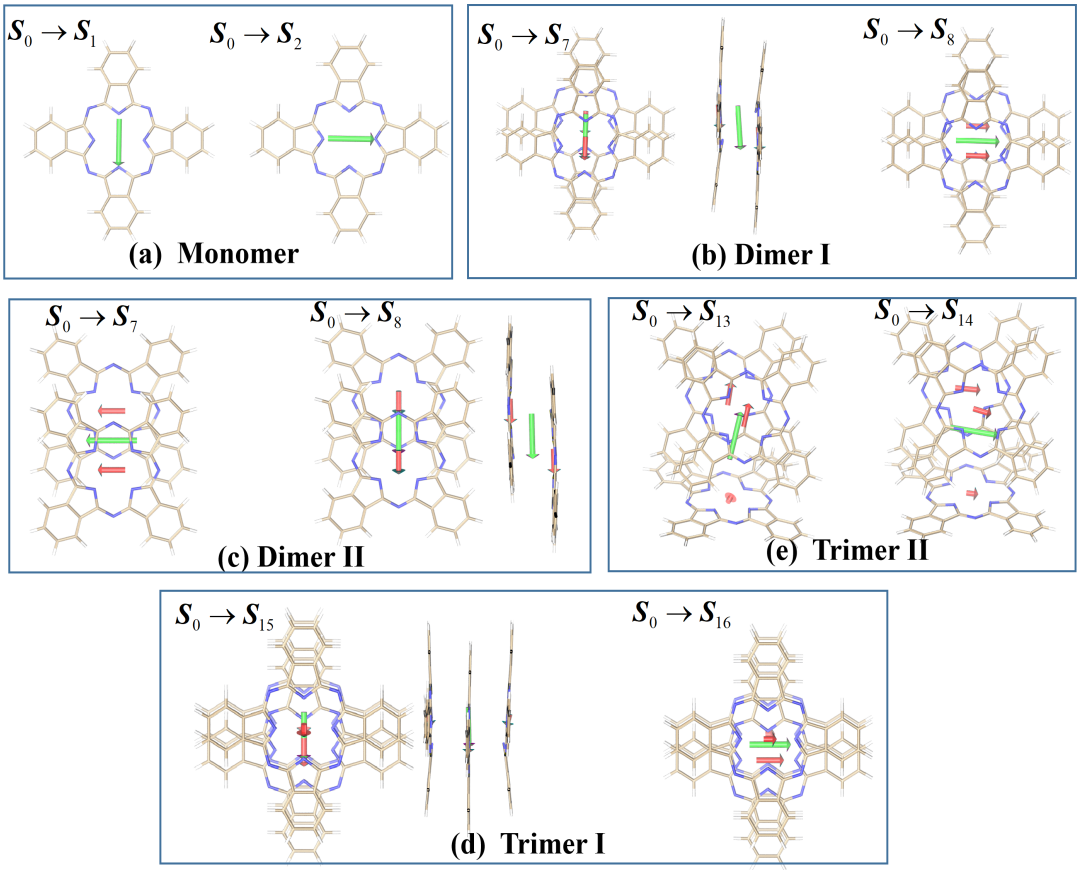


FIG. S9: Transition dipole moment vector contributed by different ZnPc monomers. The red arrows represent the contribution of each monomer, and the green arrows represent the total transition dipole moment vector of the entire system. The length of the cylindrical part of the arrow corresponds to the size of the transition dipole moment contributed by the fragment, and the direction of the arrow indicates the direction of the transition dipole moment vector.