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

Energy decomposition analysis method for intermolecular interactions with excited states

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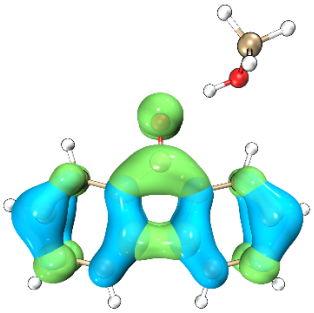
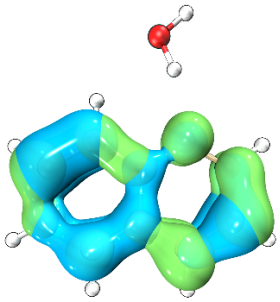
Figure S1. Electron-hole analysis results for fluorenone…CH_3OH, quinoline…H_2O, pyridine…H_2O, and benzene-TCNE, in which green color denotes the increase of electron density while blue shows the decrease of electron density (isosurface = 0.002).

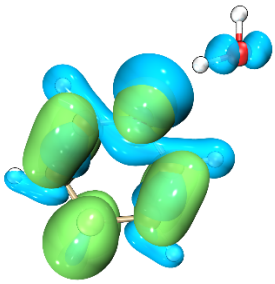
fluorenone…CH_3OH



quinoline…H_2O



pyridine…H_2O



benzene-TCNE

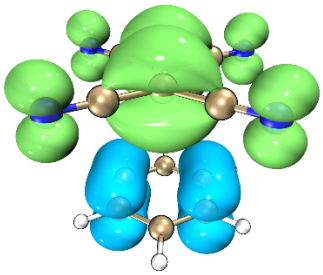


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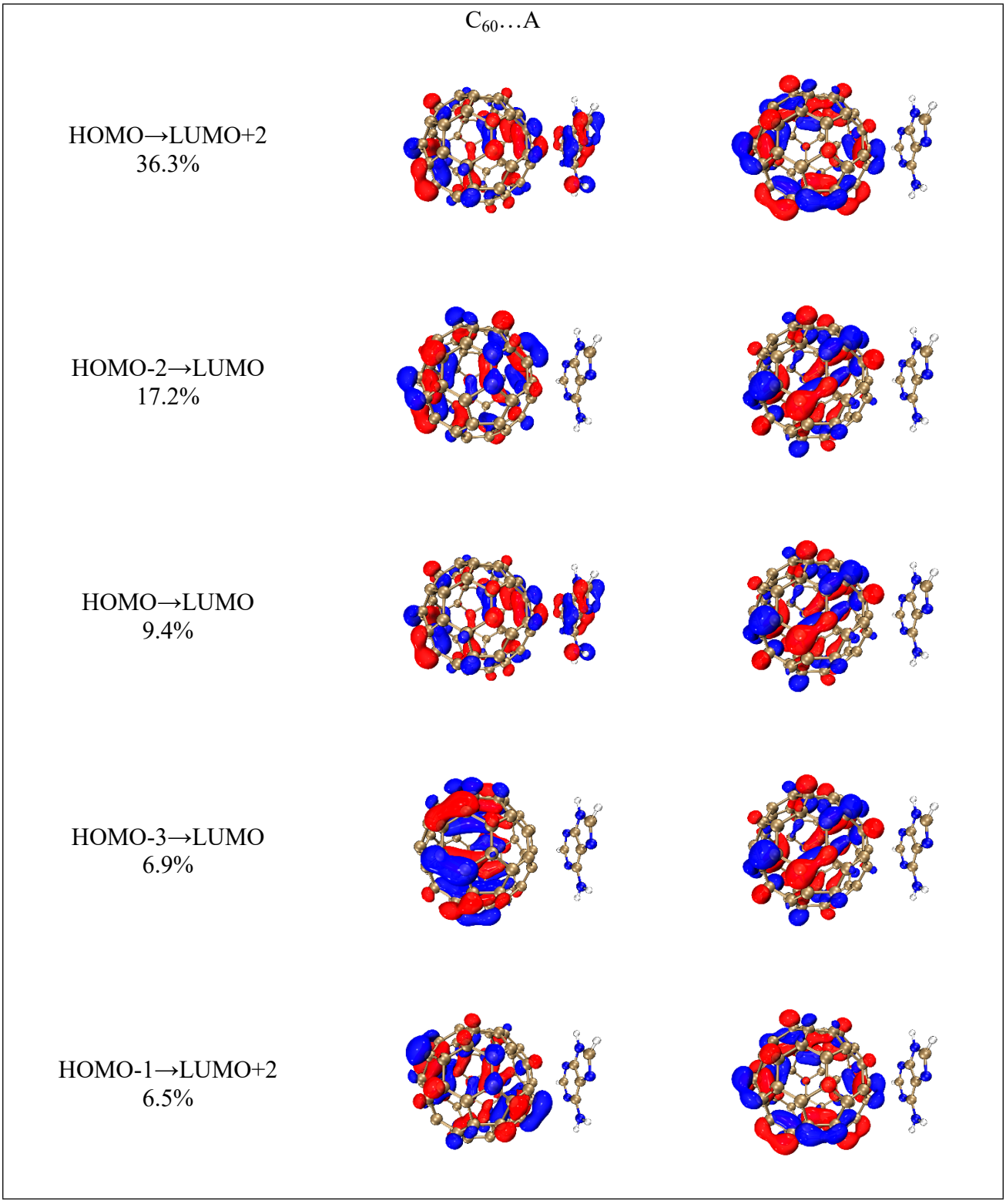
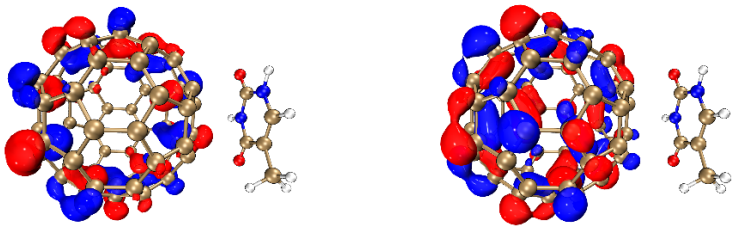
Figure S2. Orbitals involved in the transitions of C_{60}…nucleic acid bases (A, T, C and G) for the π→π* excitation.

C_{60}…A

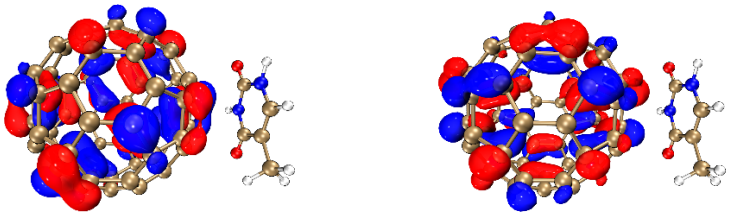


C_{60}…T

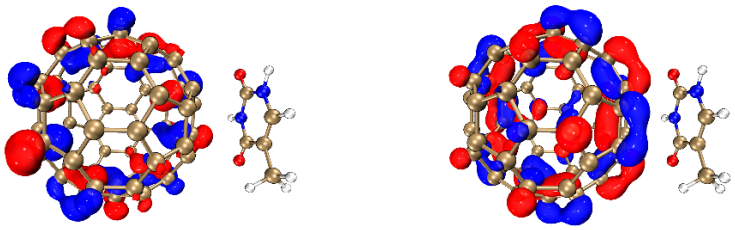
HOMO→LUMO+2
44.8%



HOMO-2→LUMO+1
26.9%



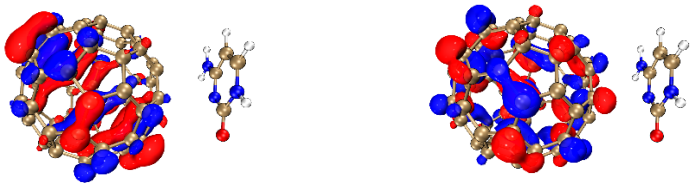
HOMO→LUMO
11.0%



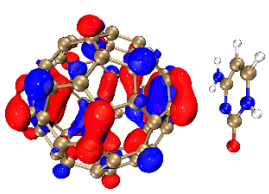
C_{60}…C

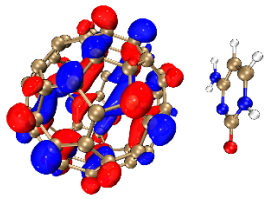
HOMO→LUMO+2
57.0%

HOMO-1→LUMO+1
21.3%

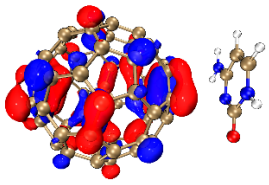


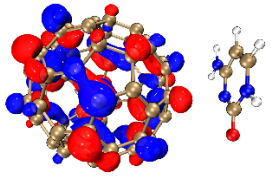
HOMO-2→LUMO
7.0%





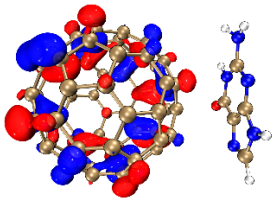
HOMO-2→LUMO+1
6.5%

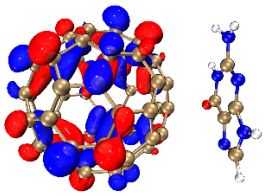




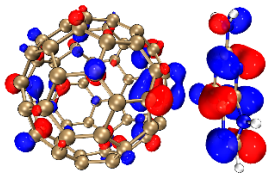
C_{60}…G

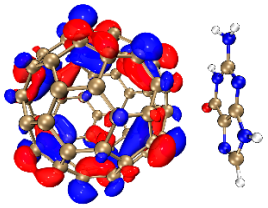
HOMO-2→LUMO+1
20.7%



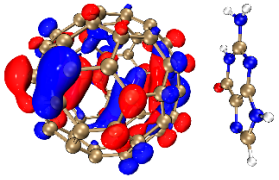


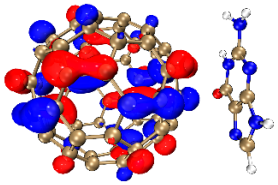
HOMO→LUMO
18.0%





HOMO-1→LUMO+2
13.7%





HOMO-5→LUMO
12.6%

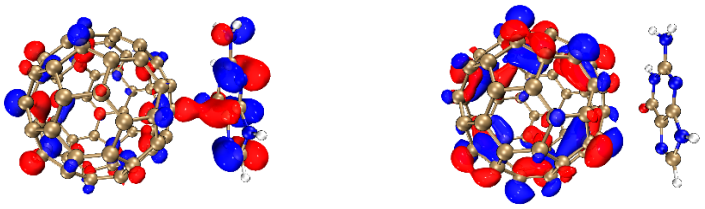


Table S1. The variation of the NPA charge Δq with the excitations computed at the CAM-B3LYP/6-311++G** level.

Complex	Monomer	Δq
fluorenone-CH_3OH	fluorenone	0.004
	CH_3OH	-0.004
quinoline-H_2O	quinoline	-0.003
	H_2O	0.002
pyridine-H_2O	pyridine	-0.029
	H_2O	0.029
benzene-TCNE	benzene	0.984
	TCNE	-0.986

Table S2. Orbital transtions of quinoline…H_2O in the $S_0 \rightarrow S_1$ transition. Basis set: 6-311++G**.

CAM-B3LYP	Contribution
(HOMO/-8.130 eV) → (LUMO/-0.781 eV)	37.21%
(HOMO/-8.130 eV) → (LUMO+1/0.233 eV)	20.70%
(HOMO-1/-8.651 eV) → (LUMO/-0.781 eV)	37.87%
(HOMO-1/-8.651 eV) → (LUMO+1/0.233 eV)	2.62%
B3LYP	
(HOMO/-6.794 eV) → (LUMO/-1.972 eV)	93.56%
(HOMO/-6.794 eV) → (LUMO+1/-0.978 eV)	0.21%
(HOMO-1/-7.318 eV) → (LUMO/-1.972 eV)	0.12%
(HOMO-1/-7.318 eV) → (LUMO+1/-0.978 eV)	3.26%

Table S2. Cartesian coordinates (in Å) of fluorenone-CH_3OH, obtained at M05-2X/6-311++G** level.

C	-0.83796799	3.25534892	0.05256500
C	-1.97136402	2.48449898	-0.18138599
C	-1.87176597	1.09915996	-0.32211801
C	-0.61530203	0.53307199	-0.21999100
C	0.53084201	1.30437005	0.01466100
C	0.42930499	2.67488098	0.15334301
H	-0.93871498	4.32710791	0.15779400
H	-2.93749595	2.96341491	-0.25588599
H	-2.74377990	0.48329300	-0.50495899
H	1.30039501	3.28961611	0.33455101
C	-0.21007600	-0.90153098	-0.32598200
C	1.27150702	-0.91042399	-0.13808399
C	2.14317989	-1.97972298	-0.14688399
C	3.49853110	-1.71825194	0.05551200
C	3.93990111	-0.41461900	0.25842601
C	3.05072904	0.66331100	0.26620001
C	1.70835400	0.40321100	0.06550600
H	1.77460599	-2.98378396	-0.30754101
H	4.21186590	-2.53030610	0.05487100
H	4.99447203	-0.23129600	0.41348800
H	3.41286397	1.66980100	0.42527401
O	-0.91905099	-1.86251795	-0.51918000
C	-3.86147904	-1.78139901	1.02527595
H	-4.87022114	-1.51581895	1.33307803
H	-3.15406895	-1.11973202	1.53485203
H	-3.66211200	-2.81077290	1.33151805
O	-3.79547000	-1.63180900	-0.38186100
H	-2.89799500	-1.85834599	-0.65096498

Table S3. Cartesian coordinates (in Å) of qunioline-H_2O, obtained at M05-2X/6-311++G** level.

C	-2.38317800	-1.42307603	0.00817200
C	-2.34178996	-0.05635700	0.01444700
C	-1.09691799	0.61818498	0.00675600
C	0.10243200	-0.13665199	-0.00428100
C	0.03388800	-1.55147099	-0.01343400
C	-1.18444002	-2.17393398	-0.00693700
H	-1.88758099	2.62997389	0.01674500
H	-3.33442092	-1.93694997	0.01323700
H	-3.25320792	0.52741098	0.02395500
C	-0.98792797	2.02760410	0.00848500
H	0.96203703	-2.10730910	-0.02665700
H	-1.23521197	-3.25398898	-0.01505700
C	1.38681400	1.76452005	-0.01264200
C	0.25003201	2.60443902	-0.00280200
H	2.37735200	2.20477891	-0.02292000
H	0.37647799	3.67719889	-0.00435600
N	1.32935405	0.45764801	-0.01152100
O	3.39653492	-1.58882403	-0.06175100
H	2.81746793	-0.80888402	-0.04466500
H	4.02584887	-1.46472800	0.64778101

Table S4. Cartesian coordinates (in Å) of pyridine-H_2O (HB), obtained at M05-2X/6-311++G** level.

C	0.81459700	-0.35048900	0.00000000
C	0.35794200	-1.66202500	0.00000000
N	0.00000000	0.70462300	0.00000000
C	-1.01101600	-1.88628400	0.00000000
H	1.06262700	-2.48078800	0.00000000
H	1.87449400	-0.12651200	0.00000000
C	-1.31226300	0.47954400	0.00000000
C	-1.86650700	-0.79336600	0.00000000
H	-1.40467300	-2.89356300	0.00000000
H	-1.94853900	1.35565200	0.00000000
H	-2.93962000	-0.91815300	0.00000000
O	2.24388400	2.47944500	0.00000000
H	2.17209500	3.43286000	0.00000000
H	1.33603200	2.13831500	0.00000000

Table S5. Cartesian coordinates (in Å) of benzene-TCNE, obtained at M05-2X/6-311++G** level.

C	1.91114604	-0.00272400	1.38989401
C	1.91114700	0.00265600	-1.38991499
C	1.91607106	-1.20842195	0.69260502
C	1.91617298	1.20566297	0.69726300
C	1.91610098	-1.20573103	-0.69728398
C	1.91614497	1.20835197	-0.69262600
H	1.90911400	-0.00482100	2.47201204
H	1.90911698	0.00475300	-2.47203302
H	1.91073596	-2.14526200	1.23272705
H	1.91093504	2.14041090	1.24099696
H	1.91086698	2.14519095	-1.23274803
H	1.91080701	-2.14047909	-1.24101806
C	-1.21727502	-0.00008600	0.67574698
C	-1.21728599	0.00013100	-0.67573500
C	-1.24112594	1.22173095	1.41890800
C	-1.24109304	-1.22213900	1.41852200
C	-1.24107397	1.22218394	-1.41850996
C	-1.24119198	-1.22168696	-1.41889405
N	-1.28532302	2.19365191	2.02580595
N	-1.28521502	-2.19425297	2.02511501
N	-1.28517306	2.19429994	-2.02510190
N	-1.28543401	-2.19360709	-2.02578902