Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Exploring the adsorption ability with sensitivity and reactivity of C_{12}-B_6N_6, C_{12}-Al_6N_6 and B_6N_6-Al_6N_6 heteronanocages towards the cisplatin drug: A DFT, AIM and COSMO analysis

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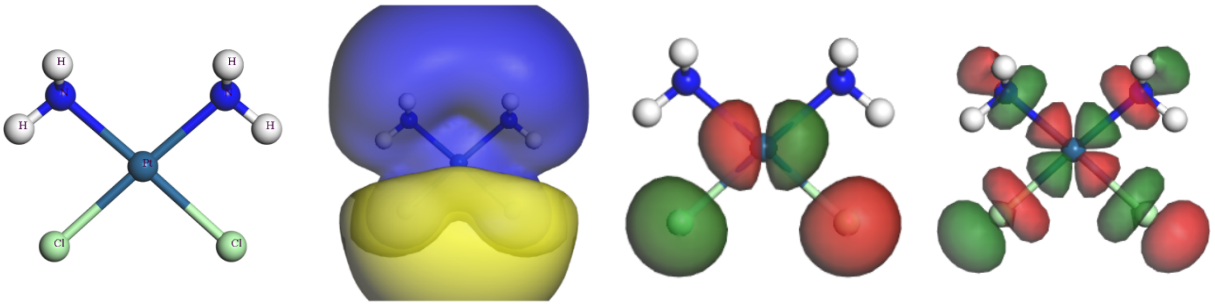


(a) (b) (c) (d)

Fig. SI1: (a) Optimized structure, (b) ESP, (c) HOMO and (d) LUMO maps of CP drug molecule.

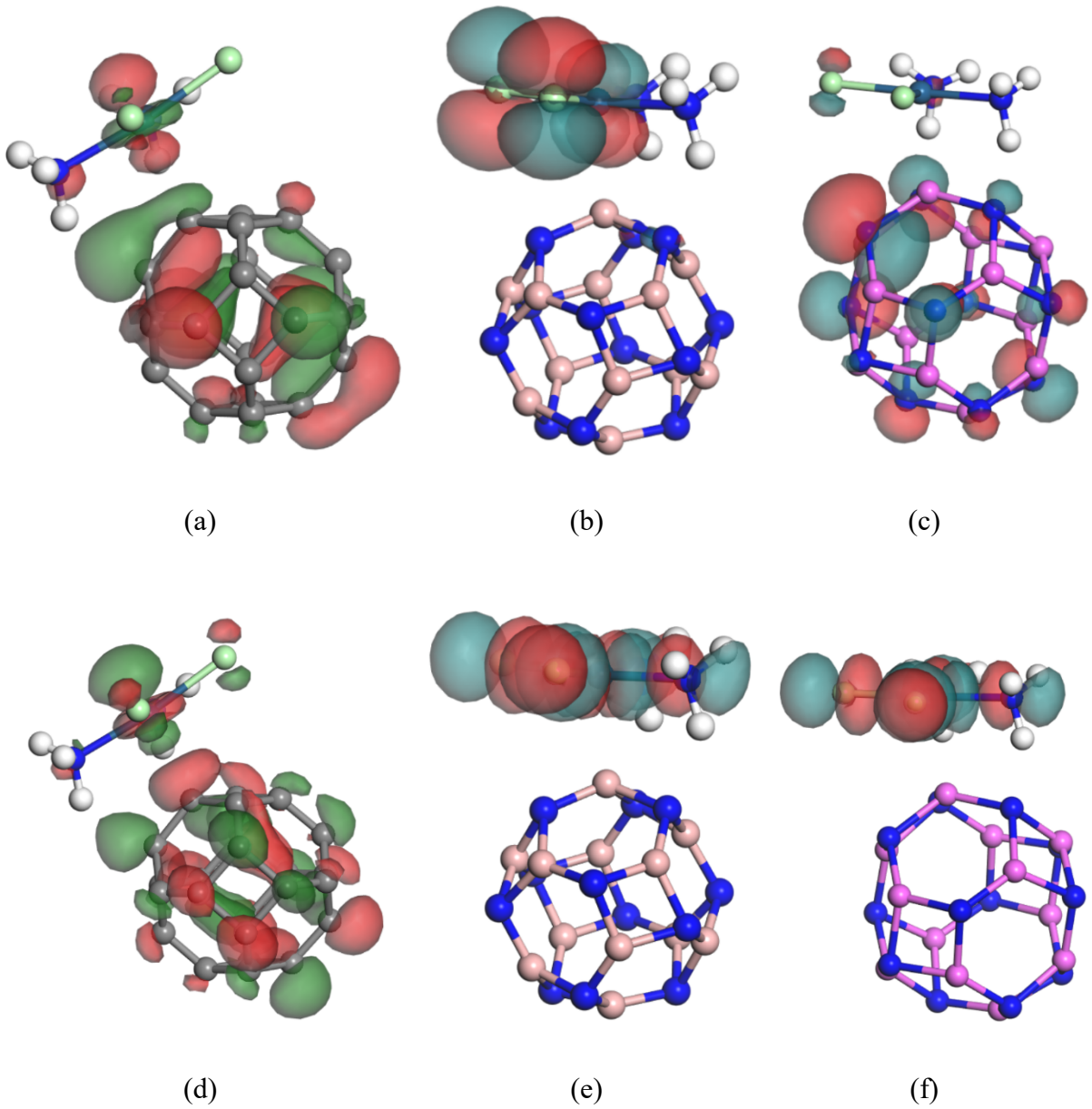
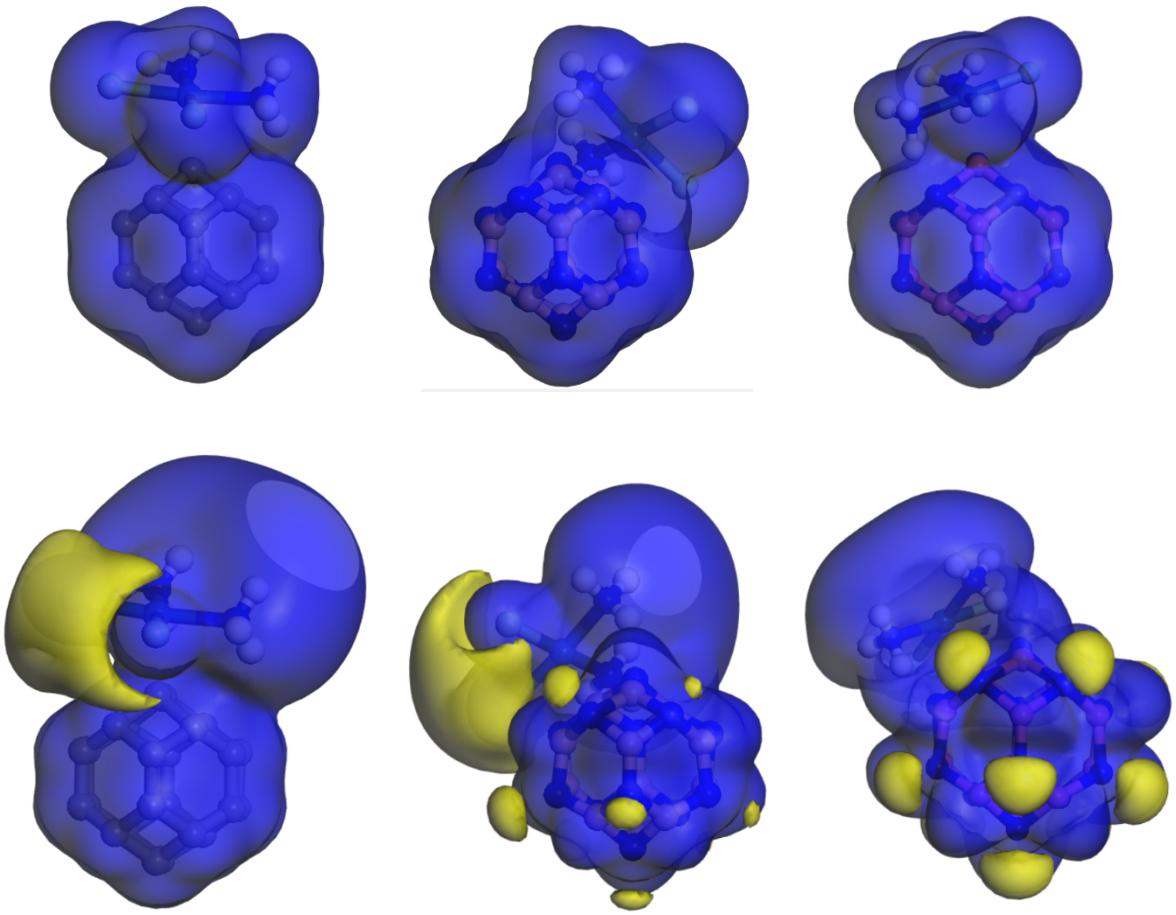


Fig. SI2: HOMO maps (a-c) and LUMO maps (d-f) of CP/C_{24}, CP/$B_{12}N_{12}$ and CP/$Al_{12}N_{12}$ complexes for S_3, S_2 and S_3 states respectively.



(a) (b) (c)

Fig. SI3: EDM (top row) and ESP (bottom row) maps of (a) CP/C_{24}, (b) CP/$B_{12}N_{12}$ and (c) CP/$Al_{12}N_{12}$ for S_3, S_2 and S_3 states respectively.

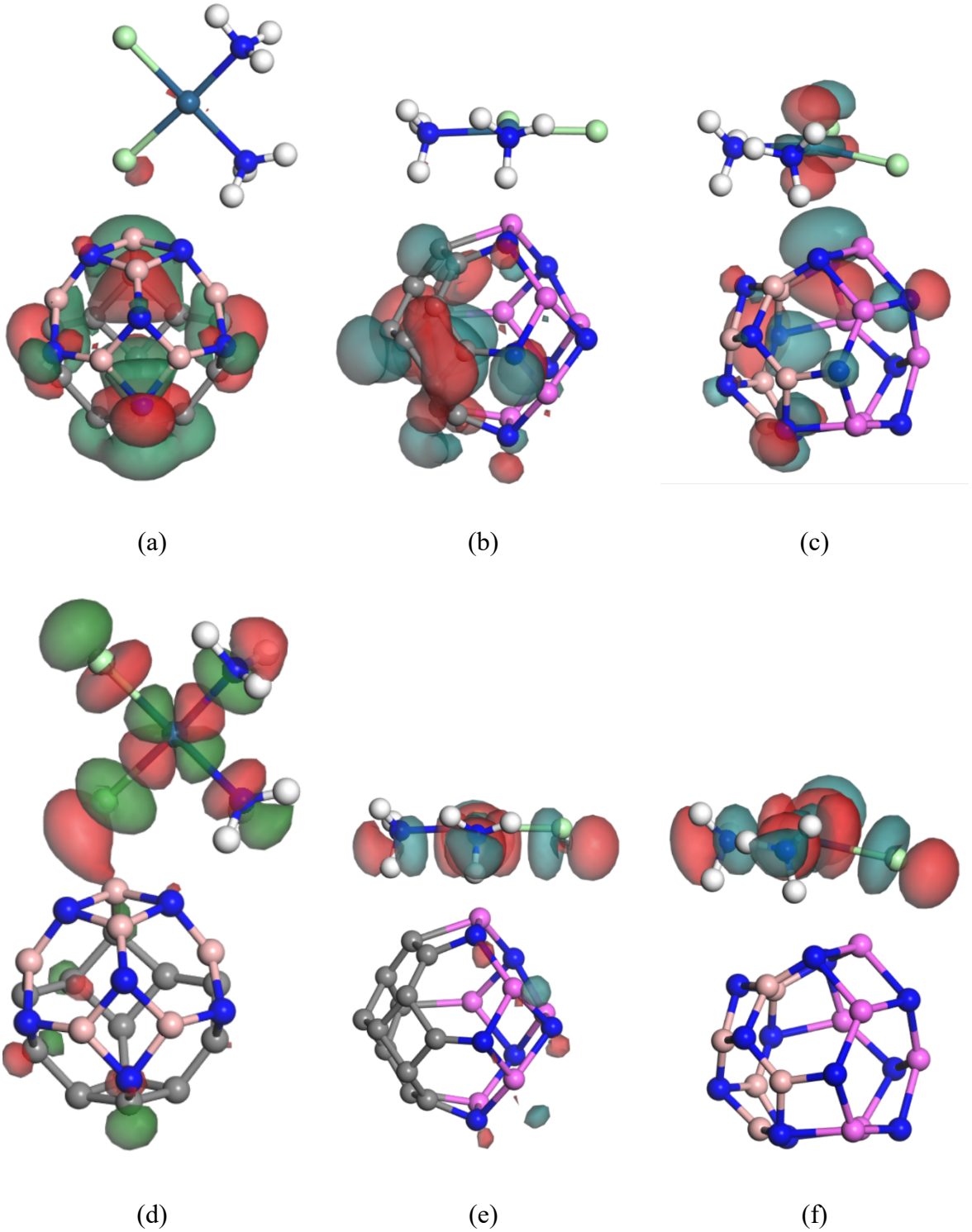
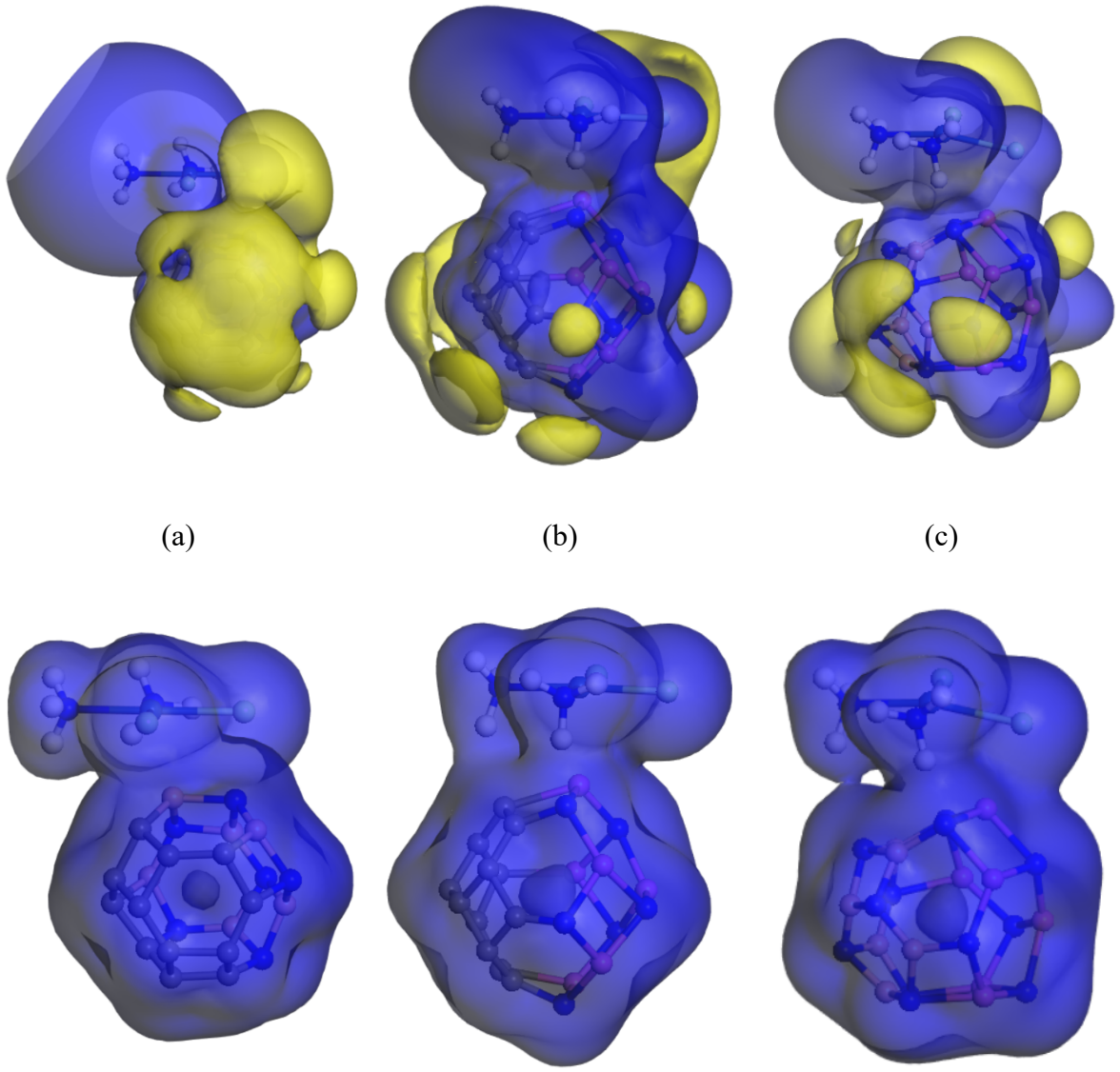


Fig. SI4: HOMO maps (a-c) and LUMO maps (d-f) of CP/C_{12}-B_6N_6, CP/C_{12}-Al_6N_6 and CP/B_6N_6-Al_6N_6 complexes of our most stable states (S_3, S_2 and S_2) respectively.



(a) (b) (c)

(d) (e) (f)

Fig. SI5: ESP (top row) and EDM (bottom row) maps of (a & d) CP/C_{12}-B_6N_6, (b & e) CP/C_{12}-Al_6N_6 and (c & f) CP/B_6N_6-Al_6N_6 for S_3, S_2 and S_2 states respectively.

Table SI1:

Fermi level energies (E_F), work function (φ) and change in work function (%φ) for CP/C_{24}, CP/$B_{12}N_{12}$ and CP/$Al_{12}N_{12}$ complexes in both gas and water phases.

Structure	State	Gas Phase			Water Phase		
		E_F (eV)	φ (eV)	% φ	E_F (eV)	φ (eV)	% φ
CP		-3.65	3.65		-3.92	3.92	
C_{24}		-5.12	5.12		-5.08	5.08	
CP/C_{24}	S1	-4.57	4.57	-10.5	-4.62	4.62	-8.8
CP/C_{24}	S2	-4.87	4.87	-4.8	-4.98	4.98	-1.9
CP/C_{24}	S3	-4.61	4.61	-9.8	-4.64	4.64	-8.6
CP/C_{24}	S4	-5.24	5.24	2.4	-5.10	5.10	0.4
$B_{12}N_{12}$		-4.62	4.62		-4.59	4.59	
CP/$B_{12}N_{12}$	S1	-4.47	4.47	-3.2	-4.28	4.28	-6.6
CP/$B_{12}N_{12}$	S2	-4.65	4.65	0.5	-4.63	4.63	0.9
CP/$B_{12}N_{12}$	S3	-4.46	4.46	-3.4	-4.29	4.29	-6.4
CP/$B_{12}N_{12}$	S4	-4.37	4.37	-5.4	-4.32	4.32	-5.7
$Al_{12}N_{12}$		-4.27	4.27		-4.45	4.45	
CP/$Al_{12}N_{12}$	S1	-4.20	4.20	-1.4	-4.32	4.32	-2.8
CP/$Al_{12}N_{12}$	S2	-4.03	4.03	-5.4	-4.19	4.19	-5.8
CP/$Al_{12}N_{12}$	S3	-4.21	4.21	-1.3	-4.33	4.33	-2.6
CP/$Al_{12}N_{12}$	S4	-4.05	4.05	-4.9	-4.17	4.17	-6.3

Table SI2:

Fermi level energies (E_F), work function (φ) and change in work function (%φ) for CP/C_{12}-B_6N_6, CP/C_{12}-Al_6N_6 and CP/B_6N_6-Al_6N_6 complexes in both gas and water phases.

Structure	State	Gas Phase			Water Phase		
		E_F (eV)	φ (eV)	% φ	E_F (eV)	φ (eV)	% φ
CP		-3.65	3.65		-3.92	3.92	

C_{12}-B_6N_6		-4.79	4.79		-4.77	4.7	
CP/ C_{12}-B_6N_6	S1	-4.36	4.36	-9.06	-4.34	4.34	-9.05
CP/ C_{12}-B_6N_6	S2	-4.44	4.44	1.97	-4.48	4.48	3.31
CP/ C_{12}-B_6N_6	S3	-4.18	4.18	-5.97	-4.25	4.25	-5.19
C_{12}-Al_6N_6		-3.98	3.98		-4.17	4.17	
CP/ C_{12}-Al_6N_6	S1	-3.94	3.94	-0.95	-4.02	4.02	-3.56
CP/ C_{12}-Al_6N_6	S2	-3.84	3.84	-2.63	-3.99	3.99	-0.86
CP/ C_{12}-Al_6N_6	S3	-3.84	3.84	0.13	-4.19	4.19	5.13
B_6N_6-Al_6N_6		-4.51	4.51		-4.72	4.72	
CP/ B_6N_6-Al_6N_6	S1	-4.55	4.55	0.99	-4.58	4.58	-3.00
CP/ B_6N_6-Al_6N_6	S2	-4.23	4.23	-7.04	-4.20	4.20	-8.27
CP/ B_6N_6-Al_6N_6	S3	-4.54	4.54	7.20	-4.59	4.59	9.47