DFT computational study of trihalogenated aniline derivative's adsorption onto nanocages

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Table S1 UV-Vis absorption values

CA

	CA	G-CA	F-CA	AiN-CA	AlP-CA	BN-CA	BP-CA
Oscillator strengths	0.1012	1.1748	0.0075	0.0036	0.002	0.1005	0.0016 0.0010
λ(max) (nm)	263	289	964	373	430	270	469 391

FA

	FA	G-A	F-FA	AlN-FA	AlP-FA	BN-FA	BP-FA
Oscillator strengths	0.0669 0.2232	1.0698	0.0076	0.0035	0.0031	0.0103	0.0011
λ(max) (nm)	253 213	289	964	376	469	216	393

BA

	BA	G-BA	F-BA	AlN-BA	AlP-BA	BN-BA	BP-BA
Oscillator strengths	0.1154	0.002	0.0081 0.0032	0.0039	0.0005	0.1023	0.0003 0.001
λ(max) (nm)	241	309	974 735	377	433	279	469 392

Table S2. Mulliken charges
CA

Molecule	Mulliken atom charges (near to cages)			Mulliken atom charges (away from NH2 group)
CA	(N4) -0.807741	(Cl1) 0.093723	(Cl2) 0.093723	(Cl3) 0.085283
G-CA	(N37) -0.673549	(Cl49) -0.011259	(Cl50) -0.011195	(Cl48) -0.017428
F-CA	(N25) -0.667146	(Cl36) -0.006483	(Cl37) -0.006875	(Cl38) -0.011364
AlN-CA	(N25) -0.729905	(Cl36) 0.041963	(Cl38) 0.035569	(Cl37) 0.021057
AlP-CA	(N25) -0.665809	(Cl37) 0.031923	(Cl38) 0.006319	(Cl36) 0.002911
BN-CA	(N25) -0.668127	(Cl36) -0.008022	(Cl38) -0.008701	(Cl37) -0.012596
BP-CA	25N -0.676724	(Cl36) -0.006955	(Cl38) -0.008093	(Cl37) -0.011850

FA

	Mulliken atom charges (near to cages)			Mulliken atom charges (away from NH2 group)
FA	(N5) -0.800779	(F1) -0.334434	(F2) -0.334437	(F3) -0.333779
G-FA	(N37) -0.662520	(F49) -0.297924	(F50) -0.301583	(F48) -0.299351
F-FA	(N36) -0.661706	(F34) -0.302214	(F35) -0.298795	(F33) -0.299265
AlN-FA	(N25) -0.716452	(F37) -0.283379	(F38) -0.273403	(F36) -0.283000
AlP-FA	(N25) -0.652184	(F36) -0.282562	(F37) -0.291777	(F38) -0.285547
BN-FA	(N25) -0.628176	(F36) -0.276197	(F37) -0.276119	(F38) -0.279273
BP-FA	(N25) -0.667361	(F37) -0.296247	(F38) -0.300679	(F36) -0.298233

BA

	Mulliken atom charges (near to NH2			Mulliken atom charges (away from NH2 group)
BA	(N4) -0.808068	(Br1) 0.145768	(Br2) 0.145766	(Br3) 0.138355
G-BA	(N40) -0.670414	(Br37) -0.107641	(Br38) -0.105086	(Br39) -0.115572
F-BA	(N25) -0.670159	(Br37) -0.111071	(Br38) -0.109366	(Br36) -0.113727
AlN-BA	(N28) -0.744913	(Br25) -0.052236	(Br26) -0.056668	(Br27) -0.083967
AlP-BA	(N28) -0.666062	(Br25) -0.092020	(Br26) 0.013552	(Br27) -0.097181
BN-BA	(N28) -0.676036	(Br25) -0.108958	(Br26) -0.078682	(Br27) -0.114555
BP-BA	(N25) -0.672237	(Br36) -0.090889	(Br38) -0.114401	(Br37) -0.108738

Table S3

Charges obtained from Natural population analysis

Cage-molecule	Cages	Molecule
AlN-CA	-0.14253	+0.14255
AlP-CA	-0.14336	+14337
BN-CA	-0.0075	+0.00749
BP-CA	-0.0035	+0.00347
F-CA	-0.00331	+0.00330
G-CA	-0.00088	+0.00288
AlN-FA	-0.14382	+0.14384
AlP-FA	-0.08338	+0.0834
BN-FA	-0.33553	+0.33553
BP-FA	-0.02039	+0.32041
F-FA	-0.00058	+0.00157
G-FA	-0.00404	+0.00346
AlN-BA	-0.19795	+0.10472
AlP-BA	-0.2275	+0.2275
BN-BA	-0.08683	+0.08685
BP-BA	-0.04880	+0.04877
F-BA	-0.01511	+0.01511
G-BA	-0.09074	+0.0108