ELECTRONIC SUPPORTING INFORMATION

Table S1: Bond distances between and 5HIAA and the doped metal of the AlNNT cages as wells the between the metal and surrounding Aluminum atoms.

Systems	Bond Labels	AlNNT-5HIAA	Bond lengths	
			Before adsorption	After adsorption
5HIAA_P@AlNNT	P100-Al38		2.2941	2.2944
	P100-Al47		2.3105	2.3081
	P100-Al45		2.2920	2.2942
	H114-P100	2.4128		
5HIAA_S@AlNNT	S100-Al38		2.3562	2.3755
	P100-Al47		2.4117	2.4393
	P100-Al45		2.2598	2.2662
	H114-S100	1.9327		
5HIAA_Si@AlNNT	Si100-Al38		2.3812	2.3705
	P100-Al47		2.4185	2.3761
	P100-Al45		2.3788	2.3586
	H114-Si100	1.9171		

Table S2: Natural bond orbital (NBO) Analysis

SYSTEMS	Transition	Donor (i)	Occupancy	Acceptor (j)	Occupancy	E(2)Kcal/mol	E(j)E(i)a.u	F(I,j)a.u
5HIAA_P@AlNNT	π– LP* (1)	π*AI $_{52}$ – N_{53}	1.90048	LP*(1) Al_{43}	0.25649	29.53	0.39	0.100
5HIAA_S@AlNNT	π– LP* (1)	π*Al_5 N_{78}	0.90491	LP*(1) Al_{77}	0.18393	22.39	0.47	0.136
5HIAA_Si@AlNNT	LP – LP*	LP (2) N_{78}	0.83319	LP*(1)Al_{77}	0.12934	30.04	0.90	0.212
P@AlNNT	π– LP* (1)	π*N_{63}-A $_{73}$	1.89967	LP*(1)Al_{64}	0.25853	29.16	0.39	0.099
S@AlNNT	LP – LP*	LP (2) N_{78}	0.83382	LP*(1)Al_{77}	0.12989	29.41	0.90	0.209
Si@AlNNT	LP – LP*	LP (1) N_7	0.83850	LP*(1)Al_5	0.13042	31.80	0.90	0.217