Adsorption of CO, SO_2, HCN, NH_3, and H_2CO on zigzag GaP nanotubes : a QM/MM study

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Electronic Supplementary Information (ESI)

RSC Adv.

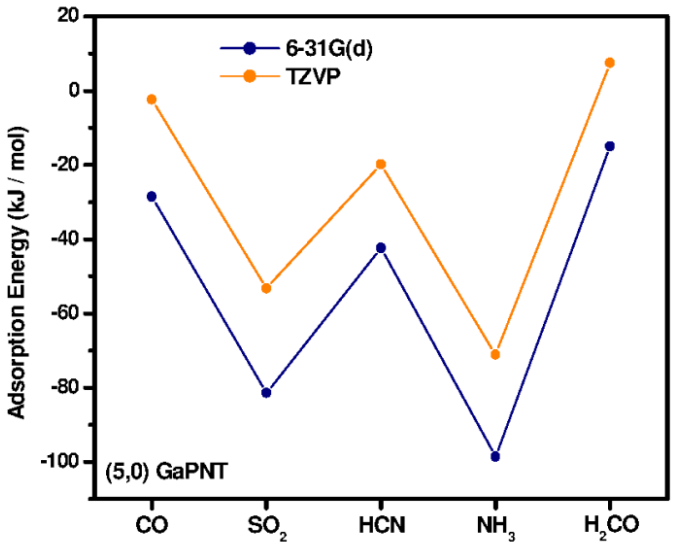

Fig. S1 Comparison of adsorption energies for (5,0)GaPNT computed with 6-31G(d) and TZVP basis sets.

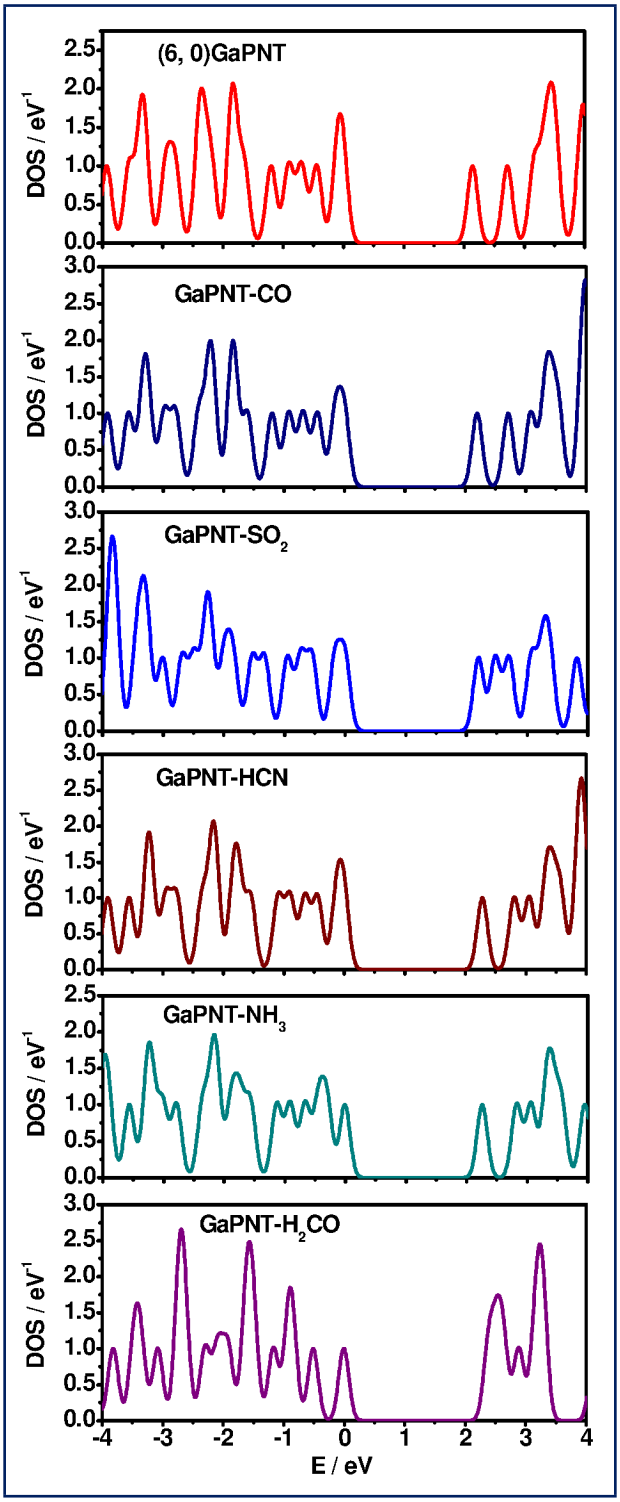

Fig. S2 Density of states (DOS) plots for the bare (6,0)GaPNT and its adsorbed complexes.

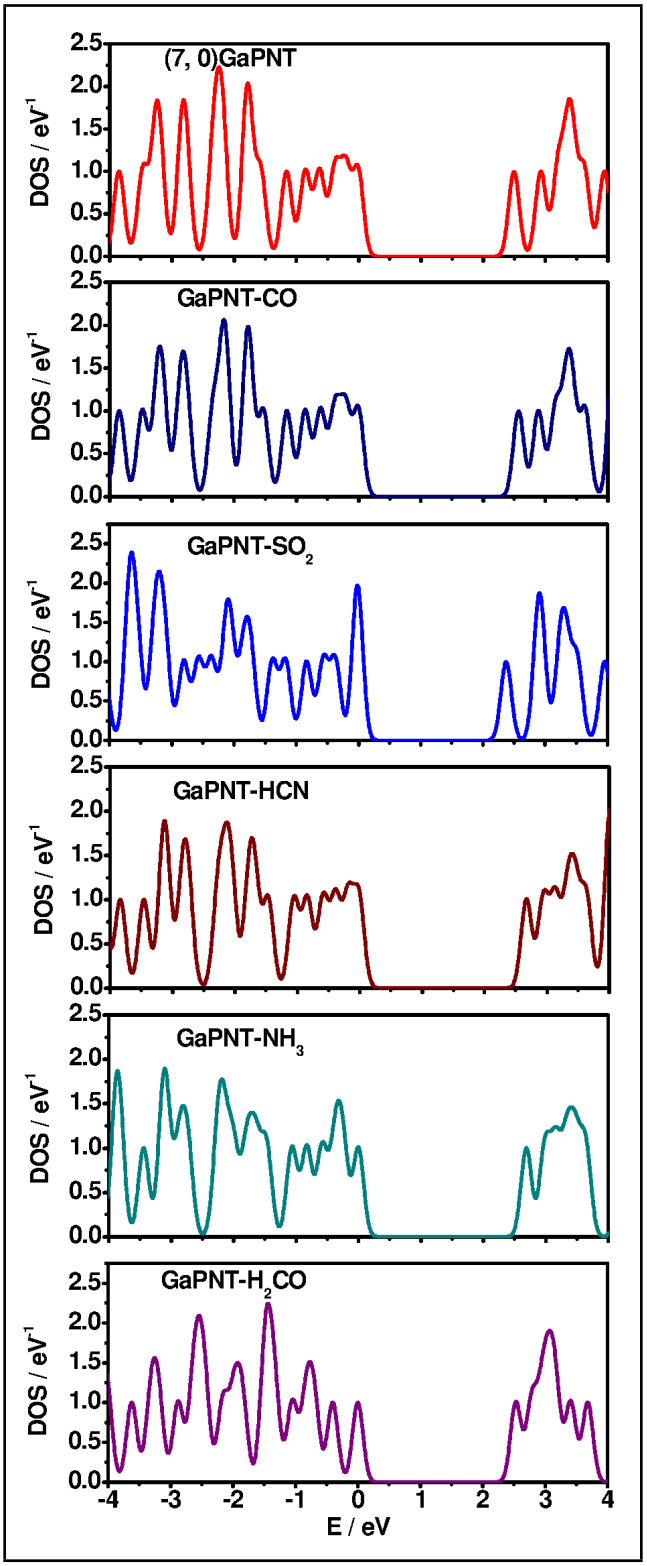

Fig. S3 Density of states (DOS) plots for the bare (7,0)GaPNT and its adsorbed complexes.

Table S1

Calculated adsorption energy (E_a) and Gibbs free energy change (ΔG_a) for the adsorption of gas molecules on (n,0)GaPNTs (n=5-7) at the ONIOM(wB97XD/6-31G(d):UFF) level of theory. All the values are in kJ/mol.

Adsorbate Molecule	(5, 0)GaPNT		(6, 0)GaPNT		(7, 0)GaPNT	
	E_a	ΔG_a	E_a	ΔG_a	E_a	ΔG_a
CO	-47.8	-11.3	-44.4	-9.5	-39.3	-4.1
SO_2	-96.3	-40.4	-88.2	-32.9	-87.2	-37.5
HCN	-71.5	-31.2	-67.0	-26.7	-51.3	-5.3
NH_3	-139.8	-99.9	-135.2	-94.9	-124.4	-84.4
H_2CO	-46.5	2.1	-46.0	2.4	-34.7	16.9

Table S2

Computed HOMO-LUMO energy gap E_g (eV) and Mulliken charge transfer (Q_T) for the most stable (n,0)GaPNT (n=5-7) adsorbate complexes at the ONIOM(wB97XD/6-31G(d):UFF) level of theory.

Adsorbate Molecule	(5, 0)GaPNT		(6, 0)GaPNT		(7, 0)GaPNT	
	E_g	Q_T	E_g	Q_T	E_g	Q_T
CO	6.74	0.19	6.77	0.17	7.02	0.15
SO_2	6.55	-0.32	6.62	-0.32	6.69	-0.32
HCN	6.81	0.17	6.85	0.18	7.13	0.18
NH_3	6.82	0.25	6.86	0.25	7.13	0.26
H_2CO	6.58	-0.37	6.68	-0.37	6.60	-0.36
Pure nanotube	6.57		6.64		6.94	