

Supporting Information

Manuscript ID: AO-2018-023407

A Density Functional study on the Adsorption of 5-membered N-heterocycles on B/N/BN doped Graphene: Coronene as a model system

Bapan Saha¹ and Pradip Kr. Bhattacharyya^{2*}

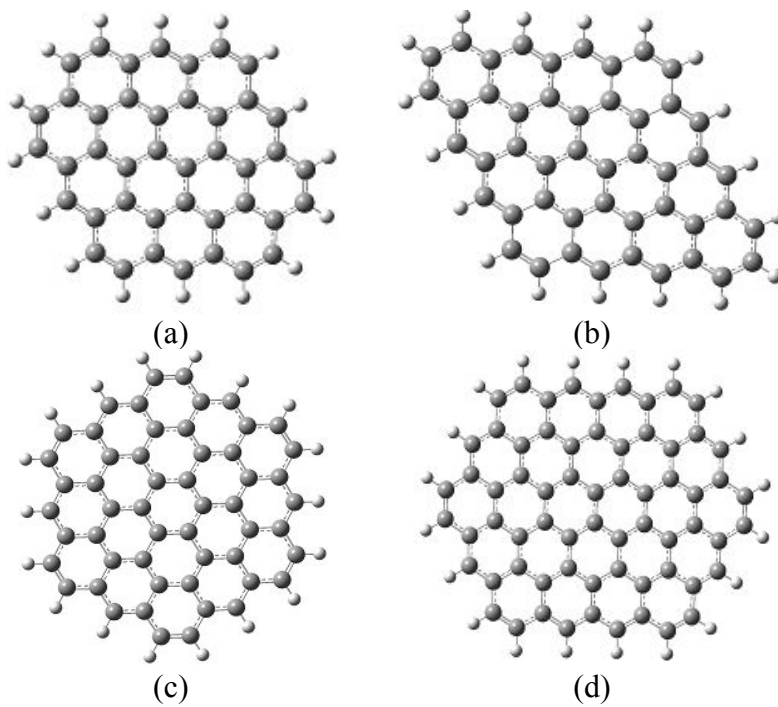
¹ Assistant Professor, Department of Chemistry, Handique Girls' College, Panbazar, Guwahati-781001, Assam, India

Email: bapan.chem@gmail.com

²Principal, Arya Vidyapeeth College, Gopinath Nagar, Guwahati-781016, Assam, India

Email: prdpbhatta@yahoo.co.in

* Corresponding author Email: prdpbhatta@yahoo.co.in (PKB)



Supporting information Figure S1 Optimized geometries of (a), $C_{42}H_{16}$, (b) $C_{48}H_{18}$, (c) $C_{54}H_{18}$ and (d) $C_{66}H_{20}$ obtained at ω B97-XD /6-311++G(d,p) level of theory

Supporting information Table S1 λ_{max} values (in nm) and corresponding excitation energies (E in eV), oscillator strengths (f) and the orbitals involved in the UV-Visible spectra of undoped/doped Cor in THF obtained at B3LYP/6-31++G(d,p) level of theory.

Systems	λ_{max}	E	f	Orbitals involved
Cor	306.8	4.04	0.98	HOMO-1→LUMO HOMO→LUMO+1
Cor _(B)	386.9	3.2	0.05	(HOMO-1)A→LUMOA (HOMO-1)B→LUMOB
	502.8	2.46	0.05	HOMOA→(LUMO+1)A (HOMO-5)B→HOMOB
Cor _(3B)	1044.9	1.18	0.01	(HOMO-3)B→HOMOB (HOMO-5)A→LUMOA
Cor _(N)	454.4	2.73	0.03	HOMOA→(LUMO+5)A (HOMO-1)B→LUMOB
	580.1	2.14	0.04	HOMOA→(LUMO+3)A (HOMO-2)B→LUMOB
Cor _(3N)	585.4	2.12	0.18	HOMOA→(LUMO+2)A HOMO-1B→(LUMO+2)B
Cor _(BN)	326.9	3.79	0.53	HOMO-1→LUMO+1 HOMO→LUMO+2
Cor _(3BN)	272.1	4.55	0.08	HOMO-1→LUMO+3 HOMO→LUMO+4
	357.1	3.47	1.85	HOMO-1→LUMO HOMO→LUMO+1

Supporting information Table S2 $\lambda_{\max}$ values (in nm) and corresponding excitation energies (E in eV), oscillator strengths (f) and the orbitals involved in the UV-Visible spectra for the complexes formed by un-doped/doped Cor in THF obtained at B3LYP/6-31++G(d,p) level of theory.

Systems	$\lambda_{\max}$	E	f	Orbitals involved
Cor-Pyr	307.6	4.03	0.86	HOMO-2→LUMO HOMO-1→LUMO+1
Cor-Im	307.5	4.03	0.87	HOMO-1→LUMO HOMO→LUMO+1
Cor-Pz	308.1	4.02	0.87	HOMO-1→LUMO+1 HOMO→LUMO
Cor-123-tria	307.7	4.03	0.89	HOMO-1→LUMO HOMO→LUMO+1
Cor-124-tria	307.7	4.03	0.88	HOMO-1→LUMO+1 HOMO→LUMO
Cor-Tetra	307.8	4.03	0.89	HOMO-1→LUMO+1 HOMO→LUMO
Cor-Penta	308.5	4.02	0.86	HOMO-1→LUMO+1 HOMO→LUMO
Cor _(B) -Pyr	486.4	2.55	0.03	HOMOA→(LUMO+1)A (HOMO-7)B→HOMOB
	1105.9	1.12	0.02	(HOMO-2)B→HOMOB (HOMO-1)B→HOMOB
Cor _(B) -Im	492.4	2.52	0.04	HOMOA→(LUMO+1)A (HOMO-6)B→HOMOB
	751.5	1.65	0.02	(HOMO-3)B→HOMOB (HOMO-2)B→HOMOB
Cor _(B) -Pz	515.1	2.41	0.02	(HOMO-6)B→HOMOB (HOMO-5)B→HOMOB
Cor _(B) -123-tria	510.8	2.43	0.05	(HOMO-6)B→HOMOB (HOMO-5)B→HOMOB
Cor _(B) -124-tria	512	2.42	0.04	(HOMO-5)B→HOMOB (HOMO-4)B→HOMOB
Cor _(B) -Tetra	390.2	3.18	0.05	HOMOA→LUMOA (HOMO-1)B→LUMOB
	500.4	2.48	0.04	(HOMO-1)A→LUMOA (HOMO-5)B→HOMOB
Cor _(B) -Penta	385.6	3.21	0.04	HOMOA→LUMOA

				(HOMO-1)B→(LUMO+1)B
	510.6	2.43	0.05	HOMOA→(LUMO+1)A
				(HOMO-5)B→HOMOB
Cor _(3B) -Pyr	1075.6	1.15	0.01	(HOMO-2)B→HOMOB
				(HOMO-1)B→HOMOB
Cor _(3B) -Im	1059.5	1.17	0.03	(HOMO-3)B→HOMOB
				(HOMO-1)B→HOMOB
Cor _(3B) -Pz	1096.5	1.13	0.005	(HOMO-2)B→LUMOB
				(HOMO-1)B→LUMOB
Cor _(3B) -123-tria	1100.7	1.13	0.003	(HOMO-2)B→LUMOB
				(HOMO-1)B→LUMOB
Cor _(3B) -124-tria	1118.6	1.11	0.004	(HOMO-2)B→LUMOB
				(HOMO-1)B→LUMOB
Cor _(3B) -Tetra	1054.9	1.17	0.005	(HOMO-3)B→HOMOB
				(HOMO-1)B→LUMOB
Cor _(3B) -Penta	1051.2	1.18	0.004	(HOMO-3)A→LUMOA
				(HOMO-3)B→HOMOB
Cor _(N) -Pyr	459.9	2.7	0.03	HOMOA→(LUMO+5)A
				(HOMO-2)B→LUMOB
	592.6	2.09	0.03	HOMOA→(LUMO+1)A
				HOMOA→(LUMO+3)A
Cor _(N) -Im	453.6	2.73	0.03	HOMOA→(LUMO+5)A
				(HOMO-1)B→LUMOB
	576.3	2.15	0.03	HOMOA→(LUMO+3)A
				(HOMO-2)B→LUMOB
Cor _(N) -Pz	457.9	2.71	0.03	HOMOA→(LUMO+5)A
				HOMOA→(LUMO+6)A
	587.2	2.11	0.03	HOMOA→(LUMO+3)A
				(HOMO-2)B→LUMOB
Cor _(N) -123-tria	455.1	2.72	0.03	HOMOA→(LUMO+6)A
				(HOMO-1)B→LUMOB
	592.6	2.09	0.03	HOMOA→(LUMO+3)A
				HOMOA→(LUMO+4)A
Cor _(N) -124-tria	456.7	2.71	0.03	HOMOA→(LUMO+6)A
				(HOMO-1)B→LUMOB
	586.1	2.11	0.03	HOMOA→(LUMO+3)A
				(HOMO-2)B→LUMOB
Cor _(N) -Tetra	446.6	2.77	0.02	HOMOA→(LUMO+7)A

				(HOMO-1)B→LUMOB
	562.1	2.21	0.03	HOMOA→(LUMO+3)A
				(HOMO-2)B→LUMOB
Cor _(N) -Penta	447.2	2.77	0.02	HOMOA→(LUMO+6)A
				HOMOA→(LUMO+7)A
	561.4	2.21	0.03	HOMOA→(LUMO+5)A
				(HOMO-2)B→LUMOB
Cor _(3N) -Pyr	591.1	2.1	0.15	HOMOA→(LUMO+2)A
				HOMOB→(LUMO+2)B
Cor _(3N) -Im	591.1	2.1	0.16	HOMOA→(LUMO+2)A
				(HOMO-1)B→(LUMO+2)B
Cor _(3N) -Pz	588.9	2.1	0.15	HOMOA→(LUMO+2)A
				(HOMO-1)B→(LUMO+2)B
Cor _(3N) -123-tria	590.3	2.1	0.14	HOMOA→(LUMO+2)A
				(HOMO-1)B→(LUMO+2)B
Cor _(3N) -124-tria	589.9	2.1	0.16	HOMOA→(LUMO+2)A
				(HOMO-1)B→(LUMO+2)B
Cor _(3N) -Tetra	994.5	1.25	0.01	(HOMO-1)A→LUMOA
				(HOMO-1)A→(LUMO+1)A
Cor _(3N) -Penta	1019.1	1.22	0.001	HOMOA→(LUMO+2)A
				HOMOA→LUMOA
Cor _(BN) -Pyr	330.8	3.75	0.37	HOMO-2→LUMO+1
				HOMO→LUMO+2
Cor _(BN) -Im	325.3	3.81	0.5	HOMO-1→LUMO+1
				HOMO→LUMO
Cor _(BN) -Pz	330.8	3.75	0.4	HOMO-1→LUMO+1
				HOMO→LUMO+2
Cor _(BN) -123-tria	329.4	3.76	0.36	HOMO-1→LUMO+1
				HOMO→LUMO+2
Cor _(BN) -124-tria	324.4	3.82	0.51	HOMO-1→LUMO+1
				HOMO→LUMO+2
Cor _(BN) -Tetra	332	3.73	0.45	HOMO-1→LUMO+1
				HOMO→LUMO+2
Cor _(BN) -Penta	332	3.73	0.21	HOMO-1→LUMO+1
				HOMO→LUMO+3
Cor _(3BN) -Pyr	355.7	3.49	0.84	HOMO-2→LUMO
				HOMO-1→LUMO+1

Cor _(3BN) -Im	275.8	4.5	0.05	HOMO-1→LUMO+2 HOMO-1→LUMO+3
	362.7	3.42	0.95	HOMO-1→LUMO+1 HOMO→LUMO
Cor _(3BN) -Pz	277.9	4.46	0.05	HOMO-1→LUMO+2 HOMO→LUMO+2
	360.7	3.44	1.03	HOMO-1→LUMO HOMO→LUMO+1
Cor _(3BN) -123-tria	276.8	4.48	0.05	HOMO-1→LUMO+3 HOMO-1→LUMO+4
	359.1	3.45	1.05	HOMO-1→LUMO HOMO→LUMO+1
Cor _(3BN) -124-tria	274.1	4.52	0.04	HOMO-1→LUMO+4 HOMO→LUMO+4
	360.2	3.44	1.04	HOMO-1→LUMO+1 HOMO→LUMO
Cor _(3BN) -Tetra	277.2	4.47	0.07	HOMO-1→LUMO+4 HOMO→LUMO+4
	359.2	3.45	1.05	HOMO-1→LUMO HOMO→LUMO
Cor _(3BN) -Penta	356.8	3.47	1.1	HOMO-1→LUMO+1 HOMO→LUMO
