Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material

Electronic and optical properties of pristine and boron-nitrogen doped graphyne nanotube

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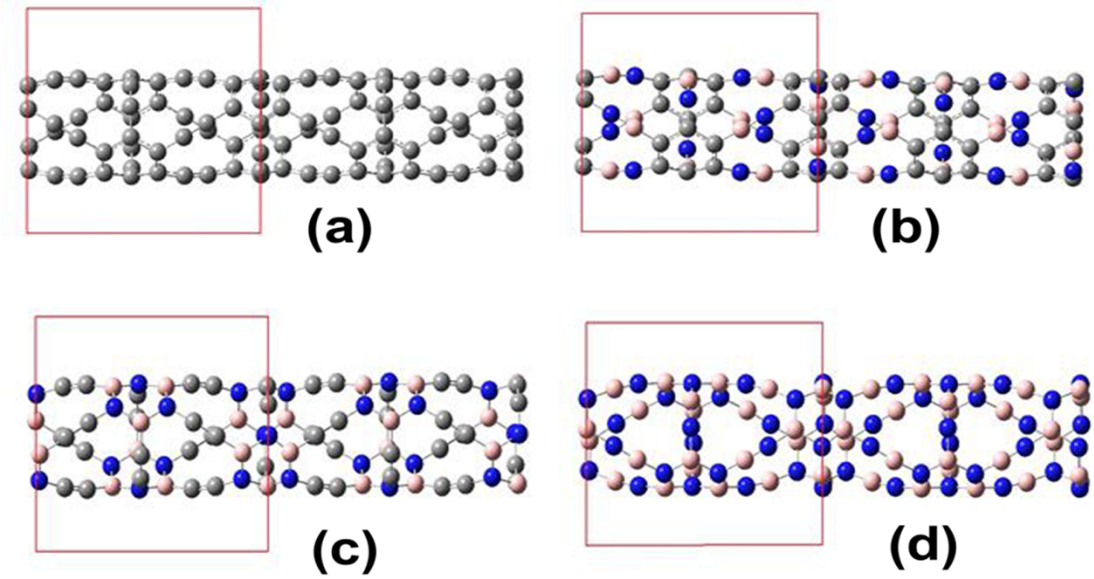

FIG. S1: Geometrical structure of (2,0) zigzag graphyne nanotube: (a) pristine; (b) graphyne with BN at chain; (c) graphyne with BN at ring; (d) graphyne like BN tube

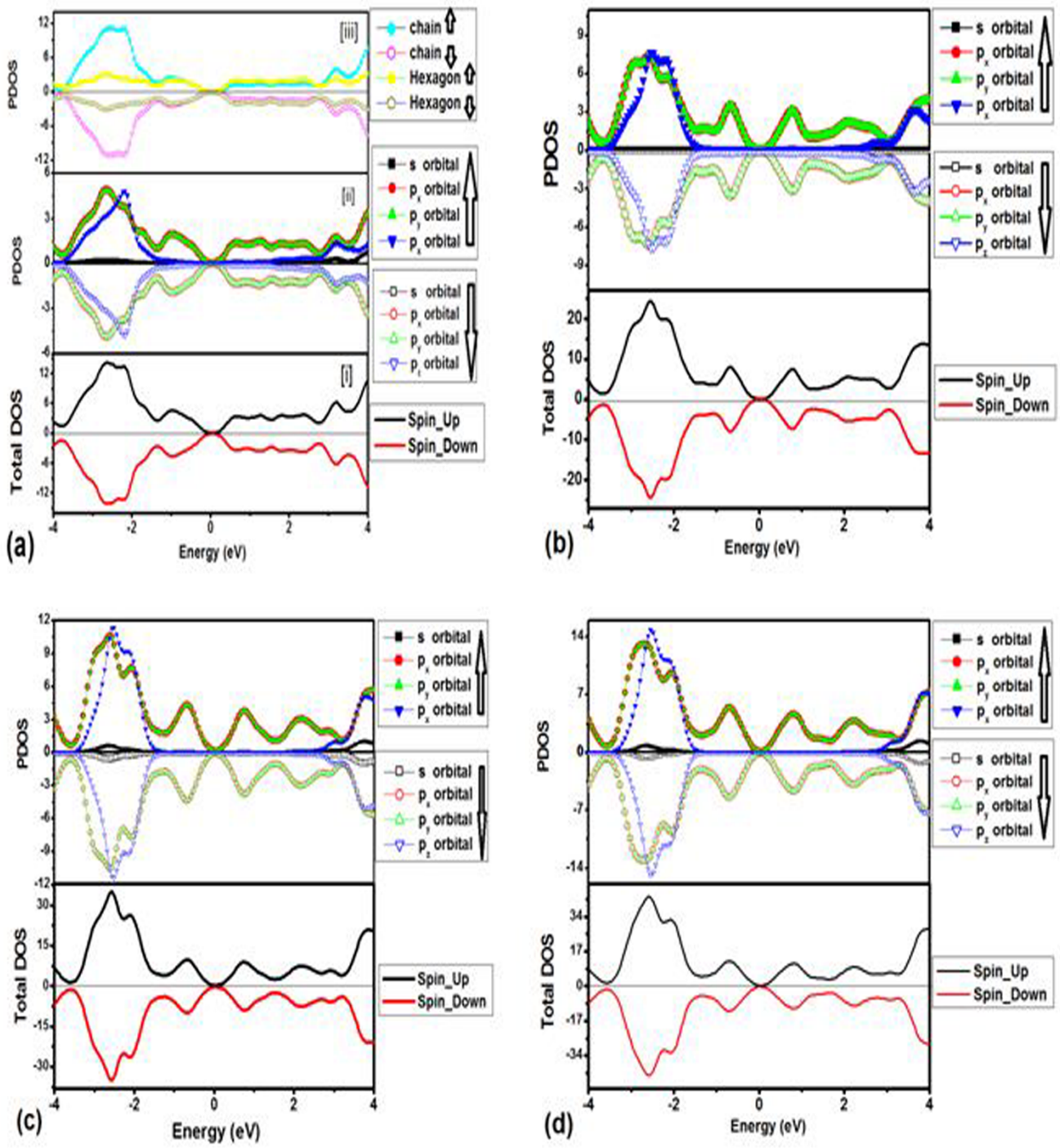

FIG. S2 A: PDOS analysis of zigzag GNT: (a) (2, 2); (b) (3,3); (c) (4,4); (d) (5,5).

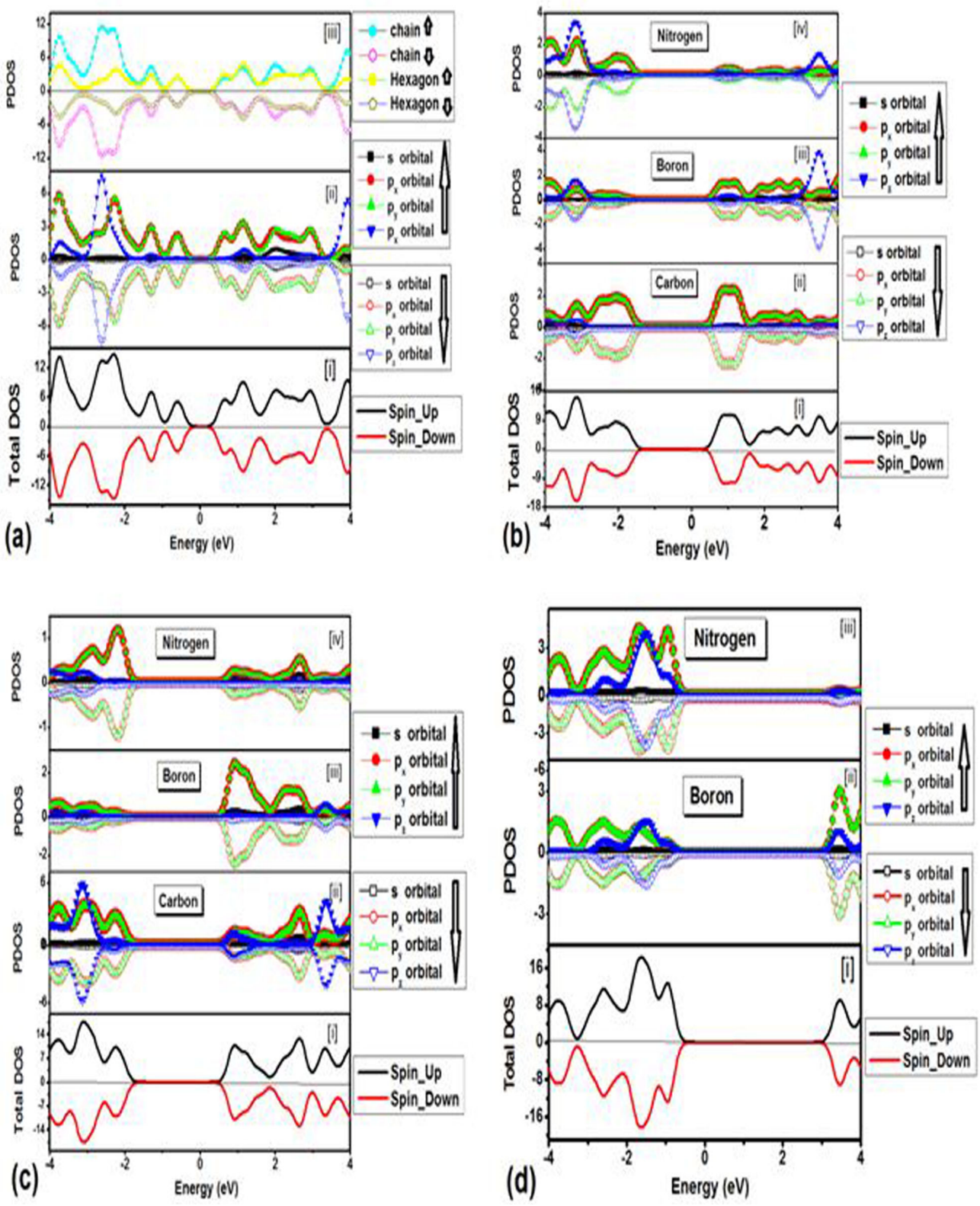

FIG. S2 B: PDOS analysis of armchair GNT: (a) (2,0) ; (b) (3,0); (c) (4,0); (d) (5,0).

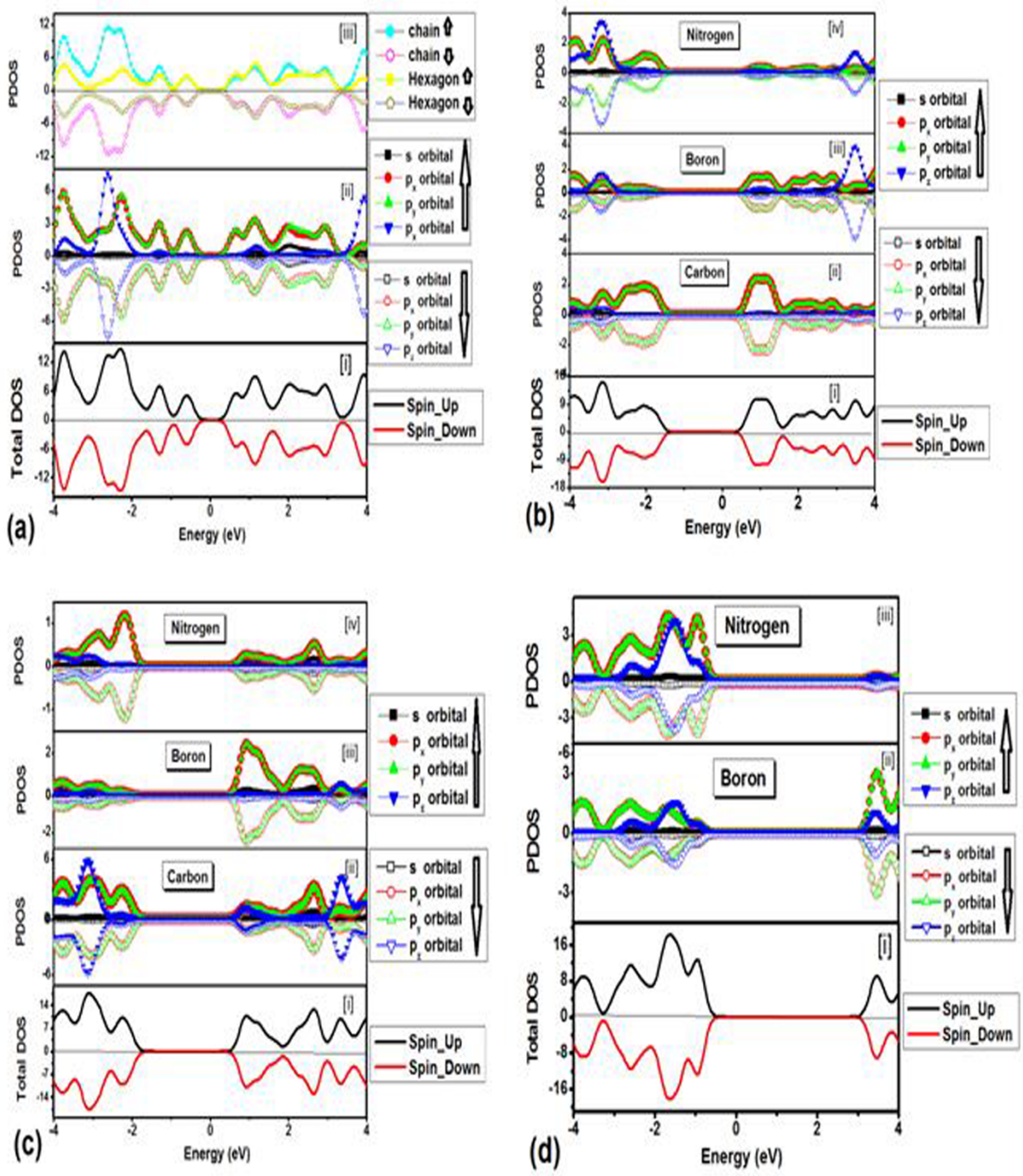

FIG. S2C: PDOS analysis of (2,0) GNT: (a) Pristine; (b) BN at chain; (c) BN at ring; (d) BNGNT

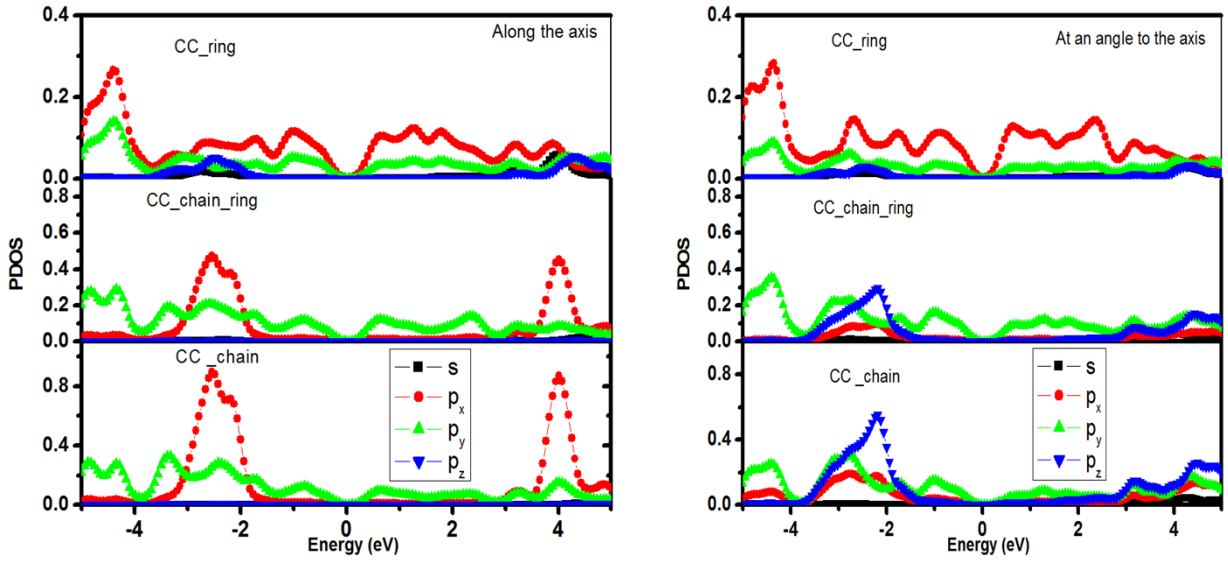

FIG. S3: PDOS analysis of pristine (2, 2) GNT in terms of the bond: (a) considering the bond parallel to the axis; (b) considering the bond at an angle to the axis.

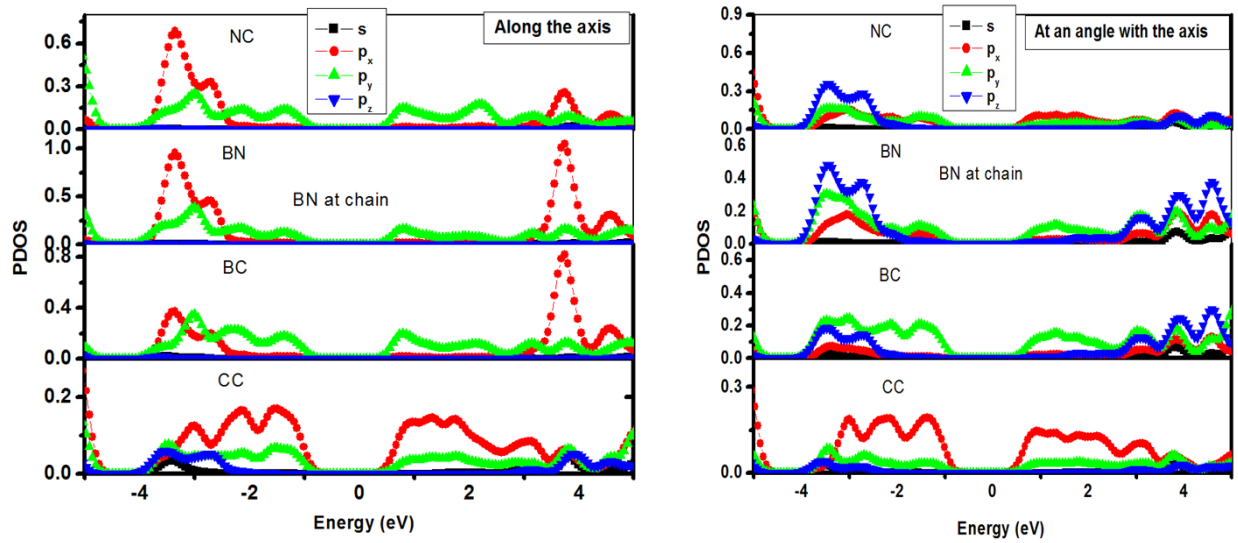

FIG. S4: PDOS analysis of (2, 2) GNT with BN at chain, in terms of bond: (a) considering the bond parallel to the axis; (b) considering the bond at an angle to the axis.

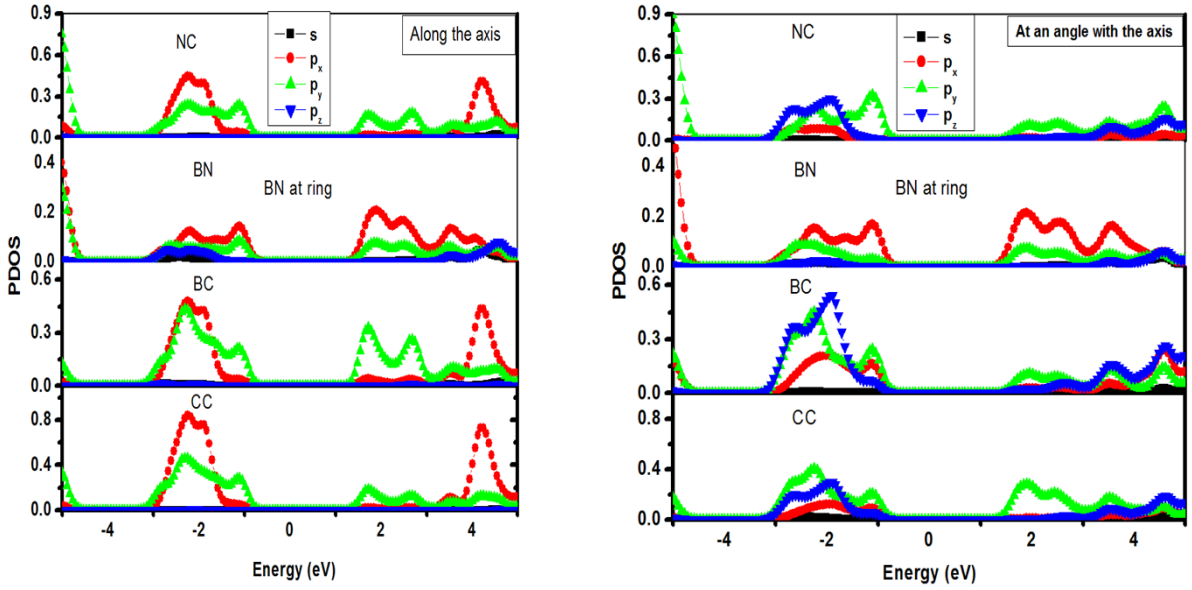

FIG. S5: PDOS analysis of (2, 2) GNT with BN at ring, in terms of bond: (a) considering the bond parallel to the axis; (b) considering the bond at an angle to the axis.

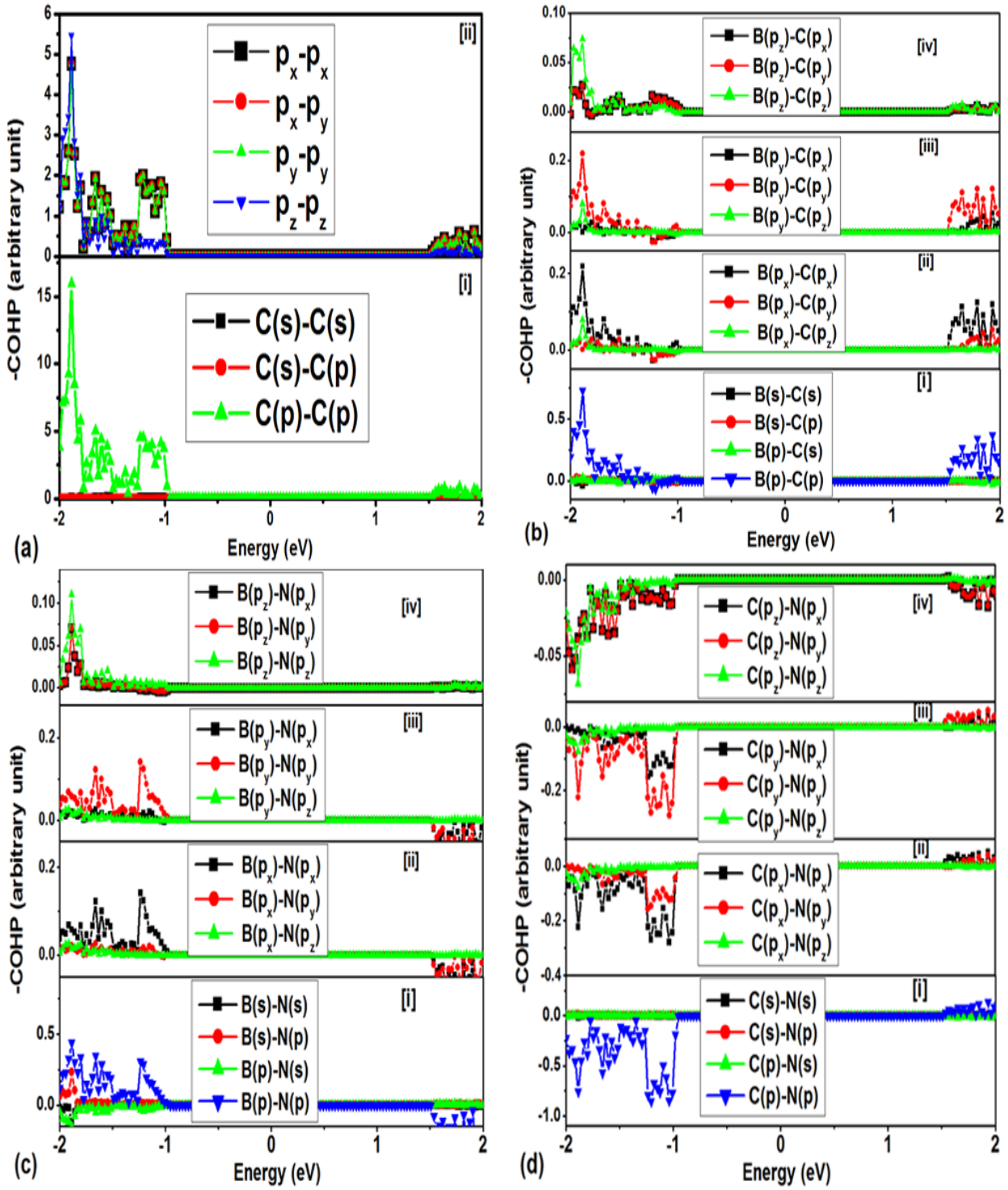

FIG. S6: -COHP analysis of (2,2) GNT with BN at ring considering; (a) C-C; (b) B-C; (c) B-N; (b) C-N interactions.

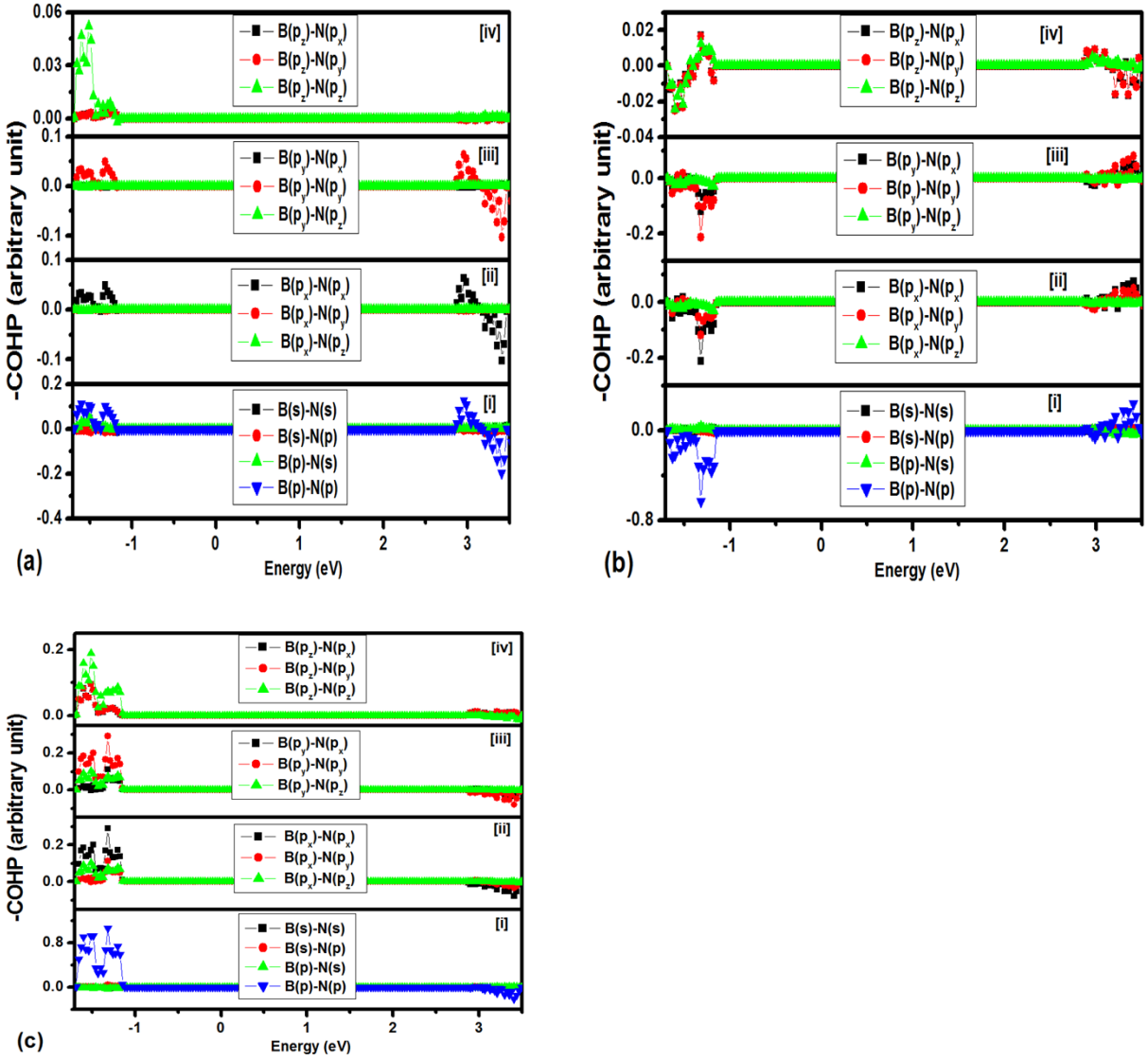

FIG. S7: -COHP analysis of (2,2) BNNT considering; (a) B-N interaction at ring (b) B-N interaction for B-N connecting chain and ring,(c) B-N interaction at chain.

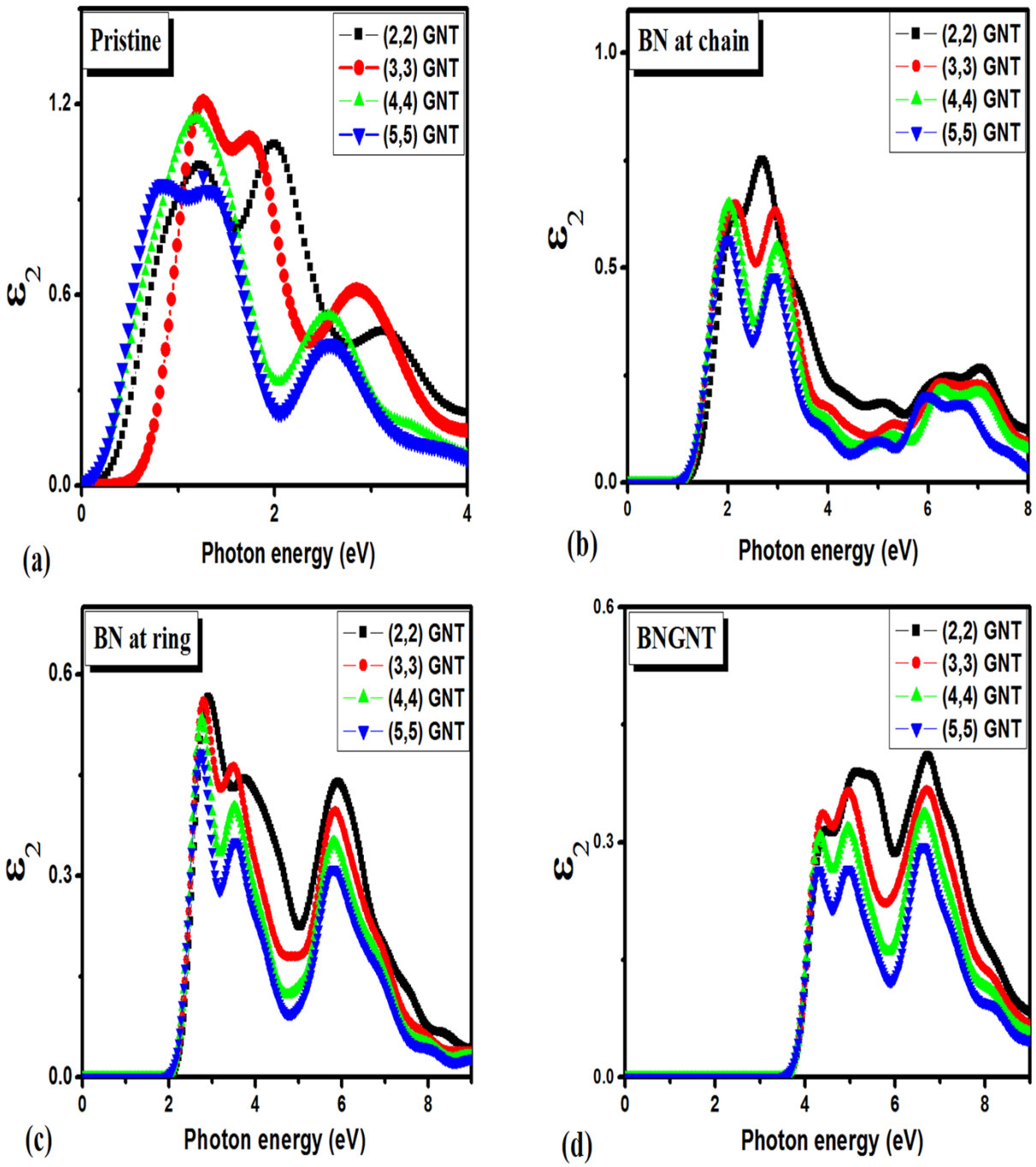

FIG. S8: Variation of first dominant peak of imaginary part of dielectric function (optical band gap) with increasing diameter: (a) pristine systems; (b) systems with BN at chain; (c) systems with BN at ring; (d) BN GNT of zigzag graphyne nanotube

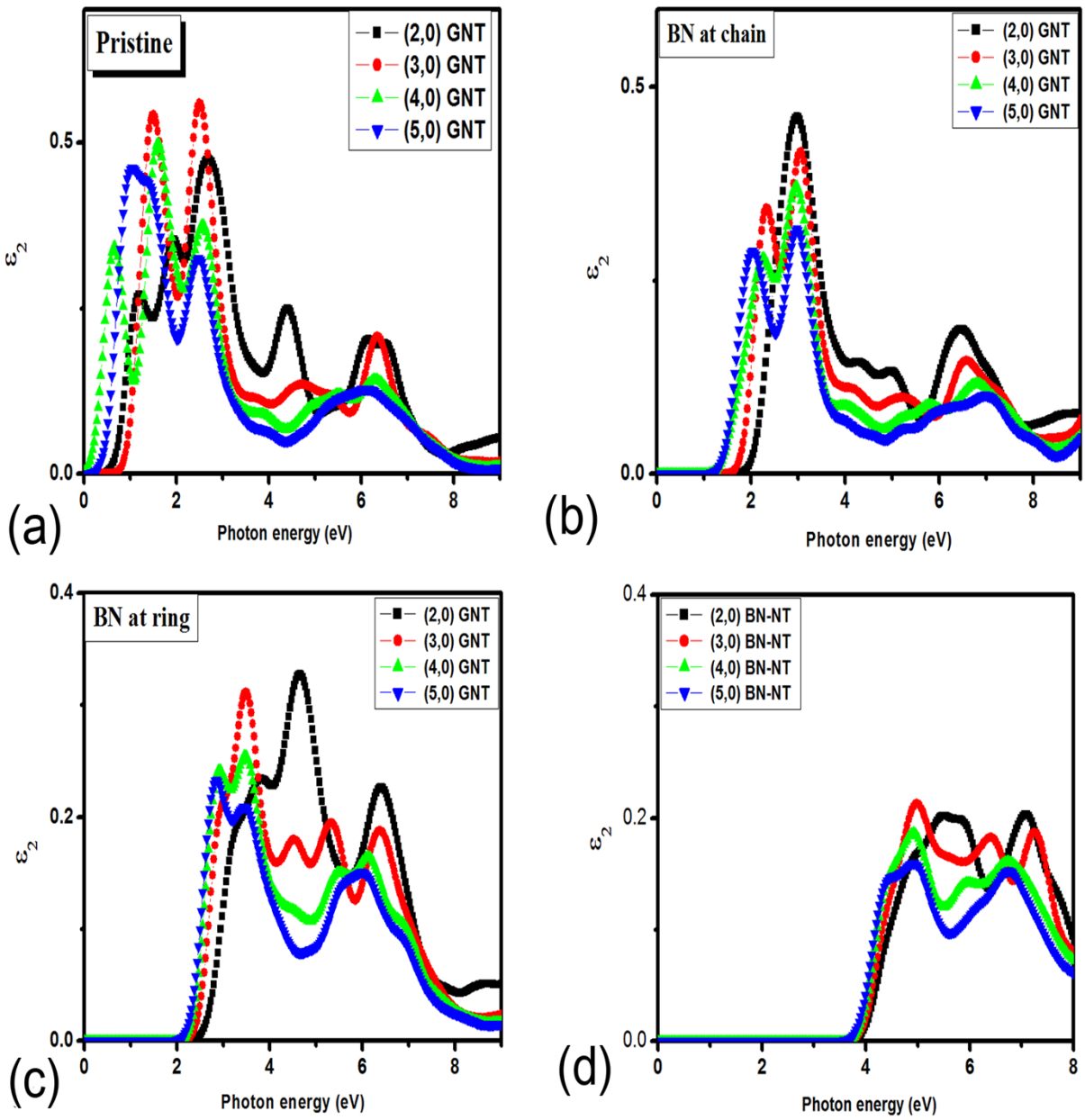

FIG. S9: Variation of first dominant peak of imaginary part of dielectric function (optical band gap) with increasing diameter: (a) pristine systems; (b) systems with BN at chain; (c) systems with BN at ring; (d) BN GNT of armchair graphyne nanotube

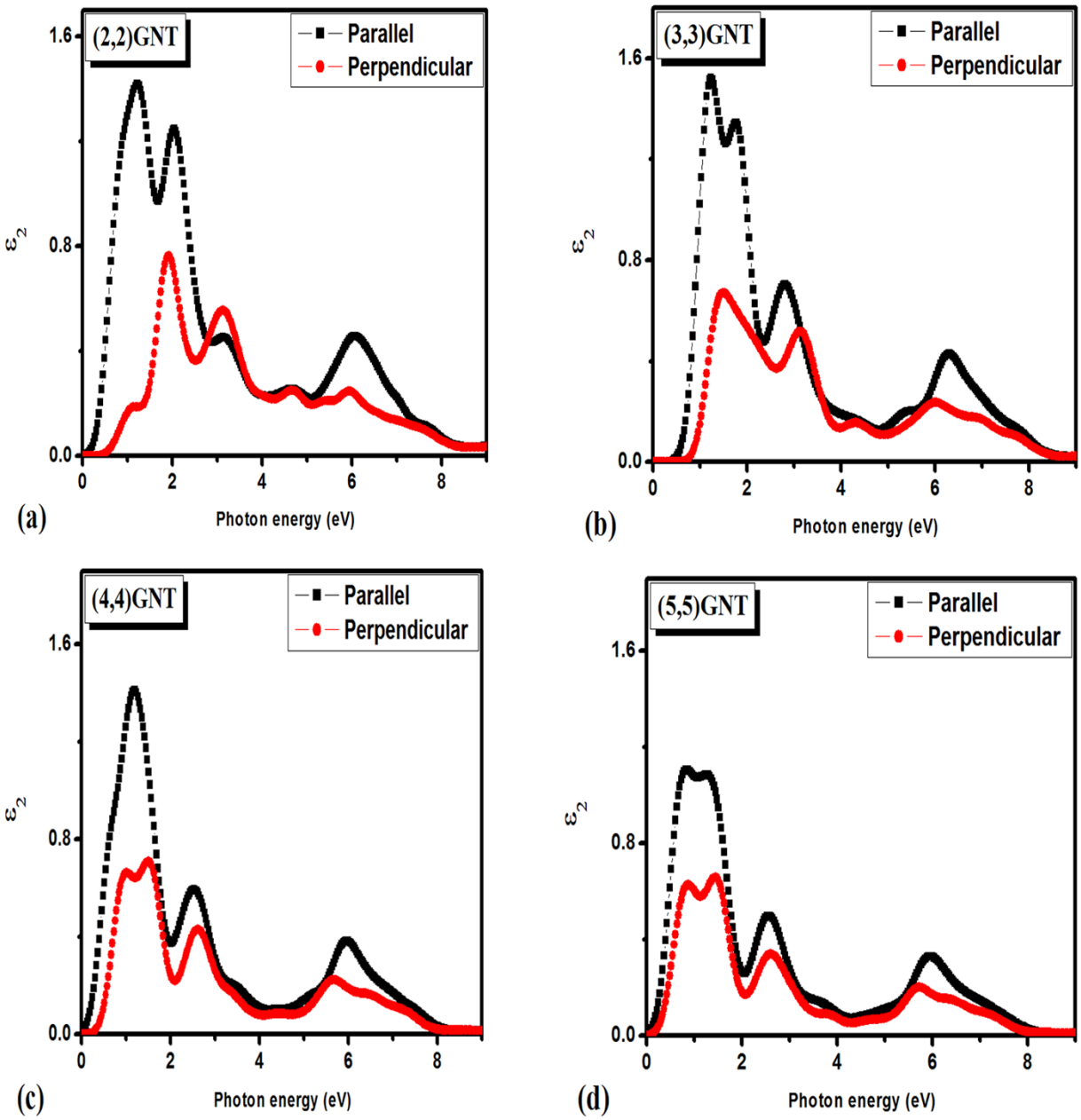

FIG. S10: The imaginary part of dielectric function of zigzag graphyne nanotube: (a) (2, 2) GNT; (b) (3, 3) GNT; (c) (4, 4) GNT; (d) (5, 5) GNT; with the incident electric filed parallel and perpendicular to the plane are displayed

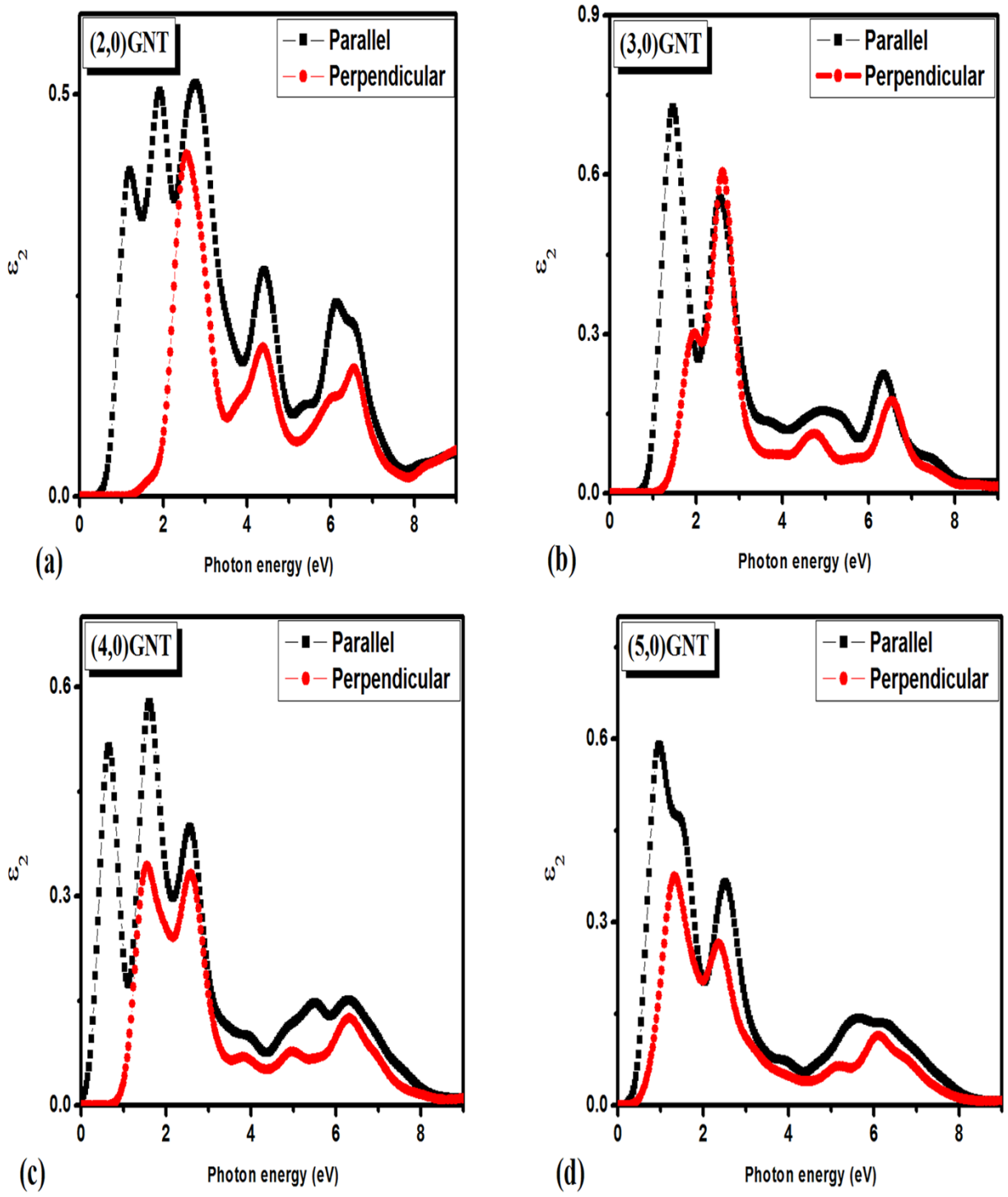

FIG. S11: The imaginary part of dielectric function of armchair graphyne nanotube: (a) (2,0) GNT; (b) (3,0) GNT; (c) (4,0) GNT; (d) (5,0) GNT; with the incident electric filed parallel and perpendicular to the plane are displayed

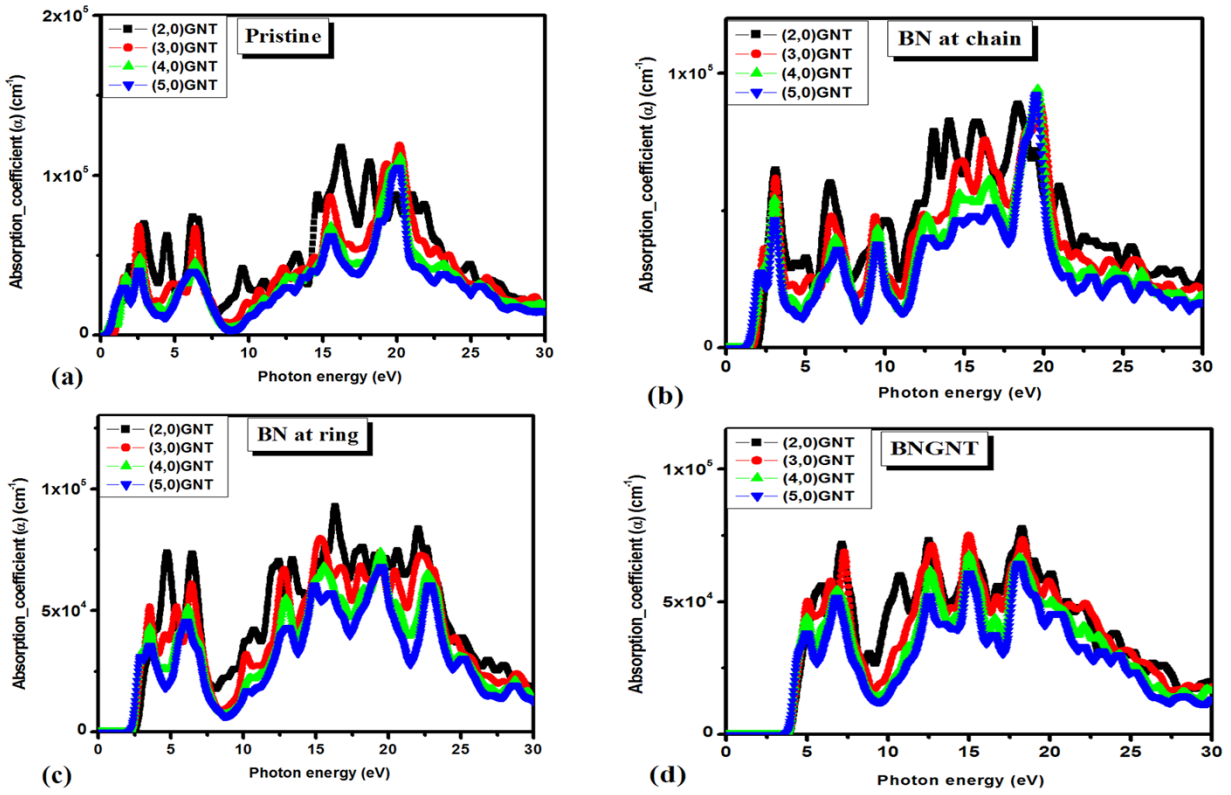

FIG. S12: Diameter dependence of absorption spectra of armchair graphyne nanotube: (a) when all four systems are pristine; (b) systems with BN at chain; (c) systems with BN at ring; (d) graphyne like BN tube

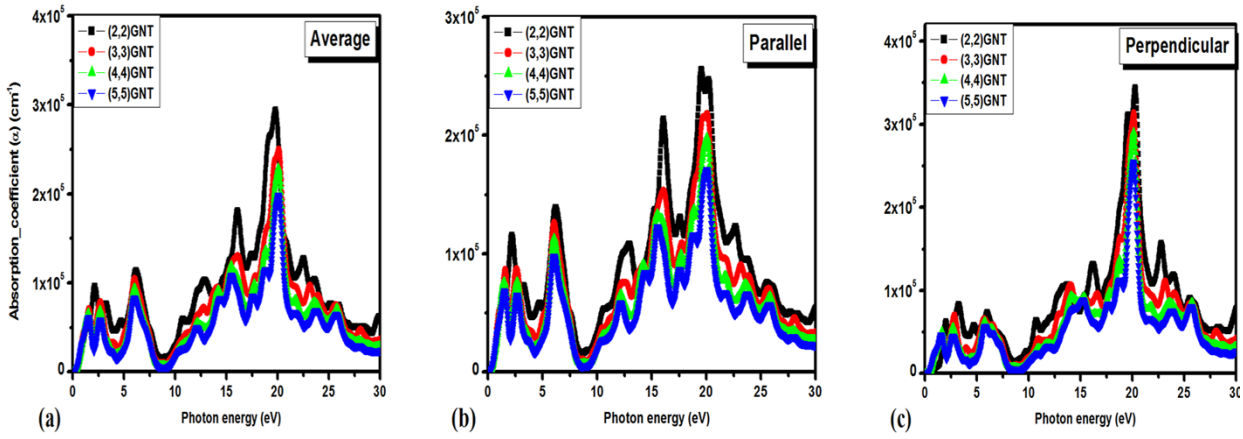

FIG. S13: Comparison of three modes of polarization of pristine (2,2) zigag graphyne nanotube: (a) average; (b) parallel polarization; (c) perpendicular polarization

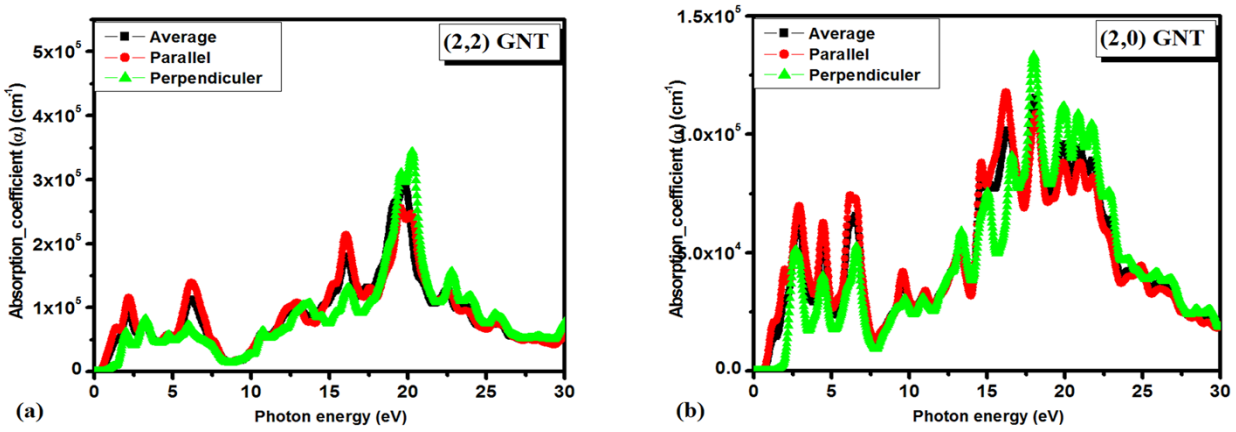

FIG. S14: Comparison of absorption spectra considering three modes of polarization of: (a) (2,2) pristine graphyne nanotube; (b) (2,0) pristine graphyne nanotube

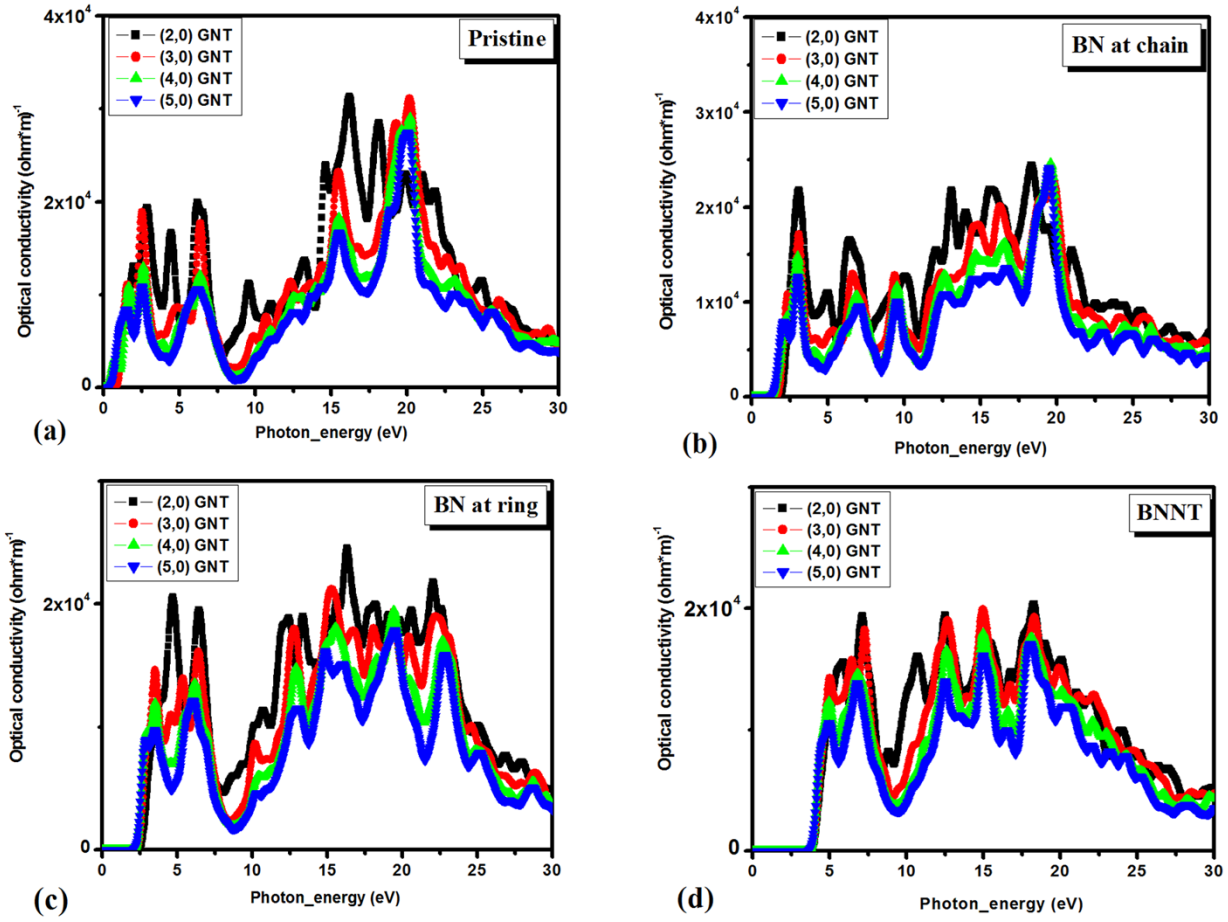

FIG. S15: Diameter dependence of optical conductivity of armchair graphyne nanotube: (a) when all four systems are pristine; (b) systems with BN at chain; (c) systems with BN at ring; (d) graphyne like BN tube

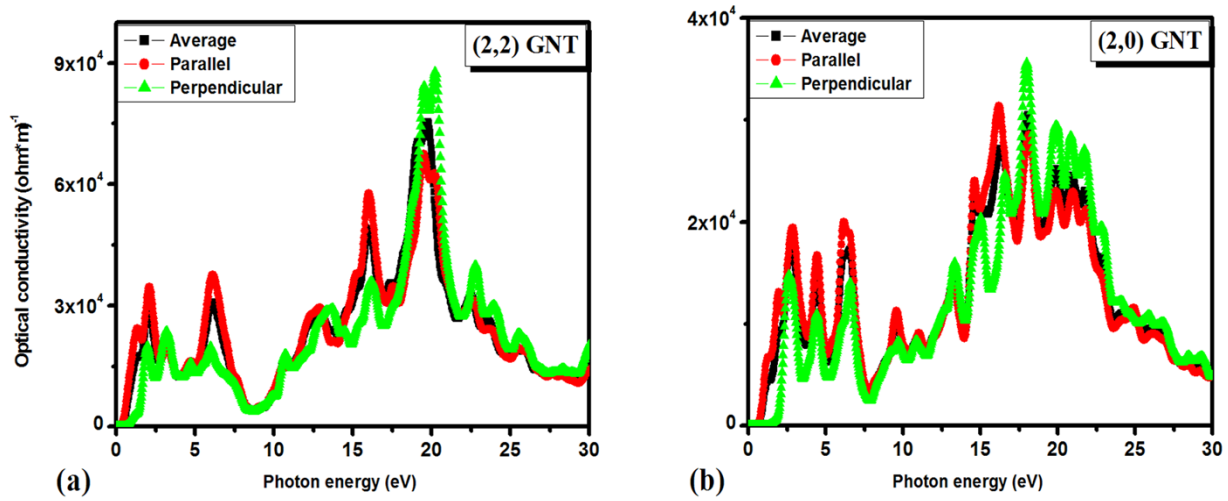

FIG. S16: Comparison of optical conductivity of considering three modes of polarization of: (a) (2,2) pristine graphyne nanotube; (b) (2,0) pristine graphyne nanotube

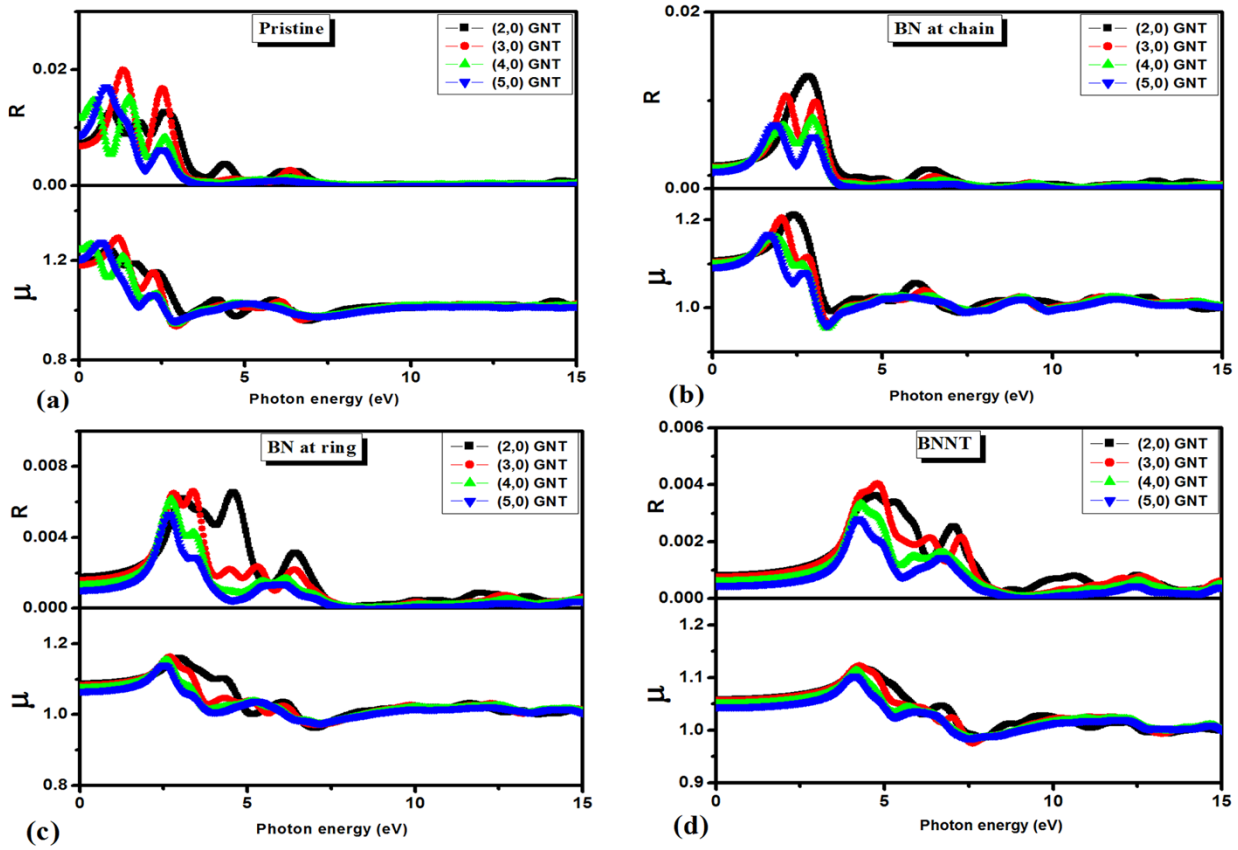

FIG. S17: Diameter dependence of reflectivity and refractive index of armchair graphyne nanotube: (a) when all four systems are pristine; (b) systems with BN at chain; (c) systems with BN at ring; (d) graphyne like BN tube

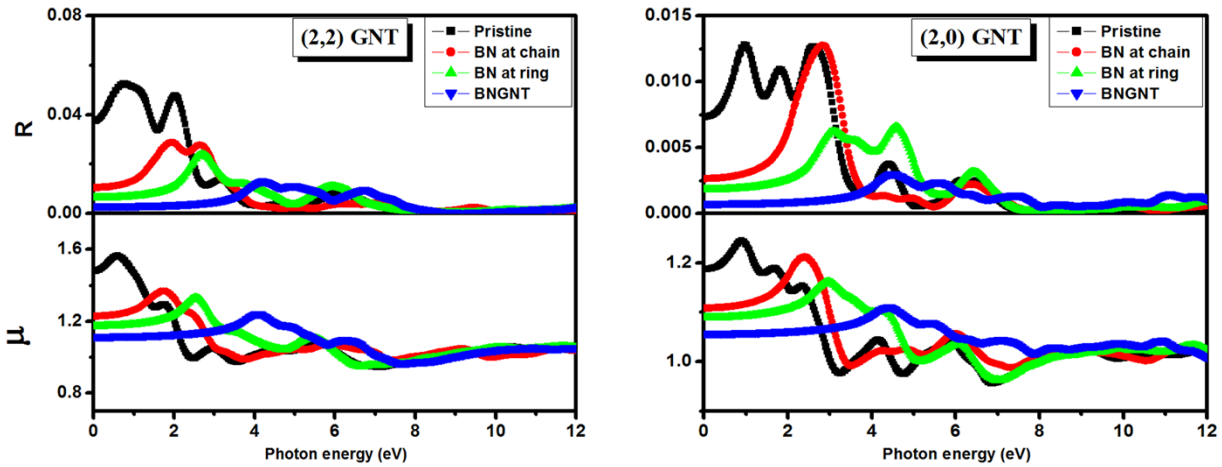

FIG. S18: Reflectivity and refractive index due to presence of BN at different site: (a) (2,2) pristine graphyne nanotube; (b) (2,0) pristine graphyne nanotube

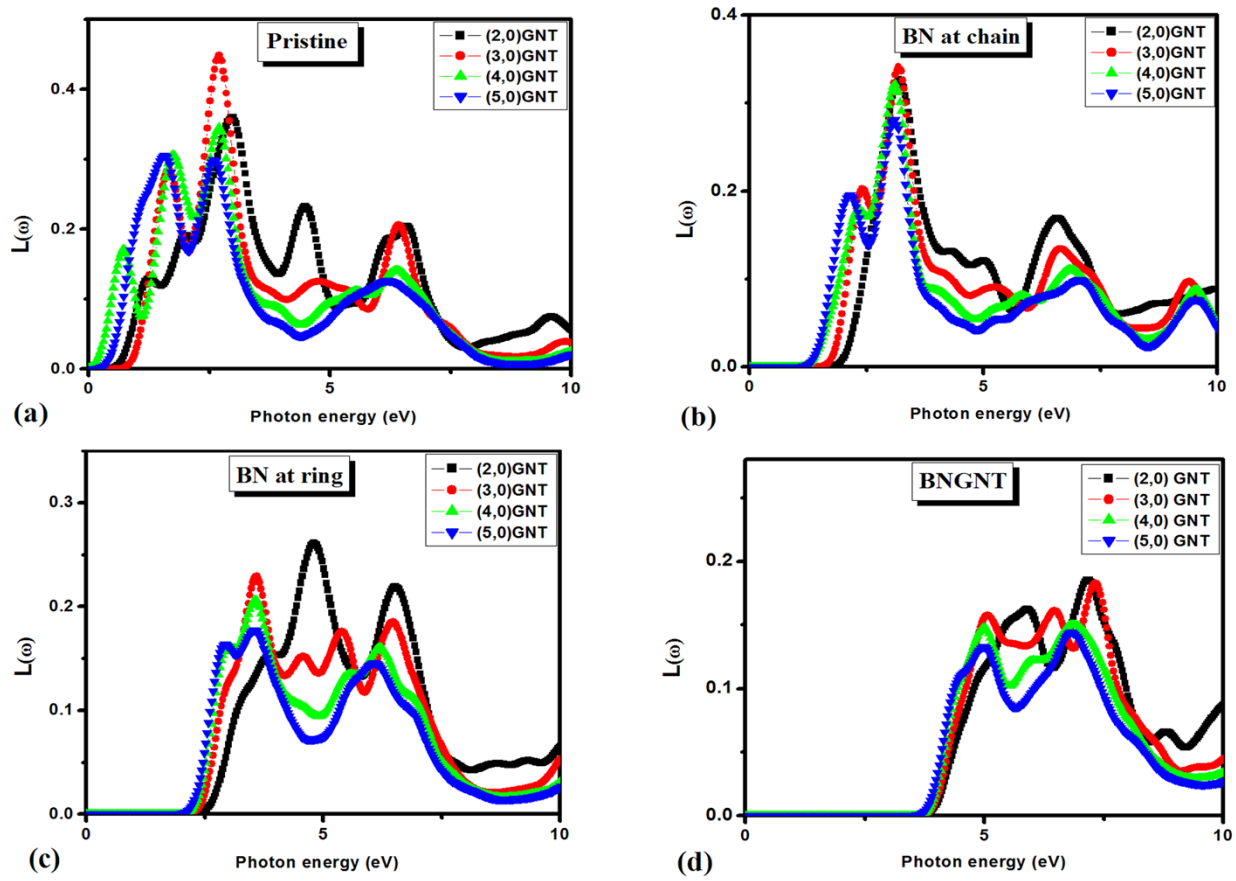

FIG. S19: Diameter dependence of energy loss function L(ω) of armchair graphyne nanotubes: (a) pristine systems; (b) systems with BN at chain; (c) systems with BN at ring; (d) graphyne like BN nanotubes.

TABLE. S1 : Magnitude of Band gap together with the Band gap location for zigzag GNT.

Systems		Band gap (eV)	Location of band gap	Nature of the semiconductor
Pristine	(2,2) GNT	0.68	X point	Direct
	(3,3) GNT	0.69	Gamma point	Direct
	(4,4) GNT	0.52	X point	Direct
	(5,5) GNT	0.53	Gamma point	Direct
GNT with BN at chain	(2,2) GNT	1.65	X point	Direct
	(3,3) GNT	1.65	VBM →Gamma , CBM→ X	Indirect
		1.67 (direct gap in Gamma)		
	(4,4) GNT	1.52	X point	Direct
	(5,5) GNT	1.56	VBM →Gamma , CBM→ X	Indirect
		1.57(direct gap in Gamma)		
GNT with BN at ring	(2,2) GNT	2.56	VBM →Gamma , CBM→ X	Indirect
		2.58(direct gap in X)		
	(3,3) GNT	2.57	VBM →Gamma , CBM→ X	Indirect
		2.59(direct gap in Gamma)		
	(4,4) GNT	2.54	VBM →Gamma , CBM→ X	Indirect
		2.54(direct gap in X)		
	(5,5) GNT	2.53	Gamma point	Direct
BNGNT	(2,2) GNT	4.08	VBM →Gamma , CBM→ X	Indirect
		4.09(direct gap in X)		
	(3,3) GNT	4.15	VBM →Gamma , CBM→ X	Indirect
		4.17(direct gap in X)		
	(4,4) GNT	4.13	VBM →Gamma , CBM→ X	Indirect
		4.14(direct gap in X)		
	(5,5) GNT	4.14	VBM →Gamma , CBM→ X	Indirect
		4.14(direct gap in Gamma)		

TABLE. S2 : Magnitude of Band gap together with the Band gap location for armchair GNT.

Systems		**Band gap (eV)**	**Location of band gap**	**Nature of the semiconductor**
Pristine	(2,0) GNT	1.08	X point	Direct
	(3,0) GNT	1.32	Gamma point	Direct
	(4,0) GNT	0.58	X point	Direct
	(5,0) GNT	0.78	Gamma point	Direct
GNT with BN at chain	(2,0) GNT	2.38	X point	Direct
	(3,0) GNT	1.95	Gamma point	Direct
	(4,0) GNT	1.67 1.69 (direct gap in X)	VBM →X, CBM→ Gamma	Indirect
	(5,0) GNT	1.64	Gamma point	Direct
GNT with BN at ring	(2,0) GNT	2.89	X point	Direct
	(3,0) GNT	2.77	Gamma point	Direct
	(4,0) GNT	2.64 2.64(direct gap in X)	VBM →X, CBM→ Gamma	Indirect
	(5,0) GNT	2.60 2.62(direct gap in X)	VBM →X, CBM→ Gamma	Indirect
BNGNT	(2,0) GNT	4.21	X point	Direct
	(3,0) GNT	4.35	X point	Direct
	(4,0) GNT	4.13	Gamma point	Direct
	(5,0) GNT	4.11	Gamma point	Direct

TABLE S3. The onset and maximum intensity with corresponding energy of E_2spectra of pristine (armchair and zigzag) GNT in the energy range 0.00-2.00 eV.

Systems	**Parallel polarization**			**Perpendicular polarization**		
	Onset of E_2	**Maximum Intensity**	**Corresponding energy (eV)**	**Onset of E_2**	**Maximum Intensity**	**Corresponding energy (eV)**
(2,0) GNT	0.50	0.51	1.92	1.35	0.06	1.98
(2,2) GNT	0.23	1.42	1.23	0.65	0.77	1.92
(3,0) GNT	0.70	0.73	1.47	1.20	0.30	1.95
(3,3) GNT	0.40	1.52	1.23	0.8	0.67	1.50
(4,0) GNT	0.10	0.58	1.59	0.90	0.34	1.56
(4,4) GNT	0.10	1.41	1.17	0.30	0.70	1.50
(5,0) GNT	0.30	0.59	1.96	0. 50	0.38	1.32
(5,5) GNT	0.10	1.09	0.90	0.20	0.66	1.44

TABLE. S4: Location of first peak and strong peak of optical conductivity of armchair GNT with its BN derivatives

Systems Pristine	Location of First peak(eV)	Location of strong peak (eV)
(2,0) GNT	1.29	16.19
(3,0) GNT	1.56	20.16
(4,0) GNT	0.72	20.18
(5,0) GNT	1.50	20.06
Systems with BN at chain		
(2,0) GNT	3.06	18.32
(3,0) GNT	2.37	19.73
(4,0) GNT	2.31	19.58
(5,0) GNT	2.10	19.47
Systems with BN at ring		
(2,0) GNT	4.67	15.65
(3,0) GNT	3.51	15.26
(4,0) GNT	3.51	19.43
(5,0) GNT	3.51	19.49
Graphyne like BN tube		
(2,0) GNT	5.84	18.26
(3,0) GNT	5.00	14.96
(4,0) GNT	4.94	14.96
(5,0) GNT	4.94	14.96

TABLE S5. Location of first peak and strong peak of optical conductivity of zigzag GNT with its BN derivatives

Systems	Location of First peak(eV)	Location of strong peak (eV)
Pristine		
(2,2) GNT	1.38	19.74
(3,3) GNT	1.5	20.07
(4,4) GNT	1.38	21.75
(5,5) GNT	1.44	23.73
Systems with BN at chain		
(2,2) GNT	2.76	18.98
(3,3) GNT	2.22	19.43
(4,4) GNT	2.07	19.34
(5,5) GNT	2.04	19.07
Systems with BN at ring		
(2,2) GNT	2.97	22.67
(3,3) GNT	2.85	19.55
(4,4) GNT	2.79	19.46
(5,5) GNT	2.76	19.37
Graphyne like BN tube		
(2,2) GNT	5.52	18.26
(3,3) GNT	4.44	18.08
(4,4) GNT	4.35	18.02
(5,5) GNT	4.32	18.06