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

Supporting Information for Tunable electronic properties of partially edge-hydrogenated armchair boron-nitrogen-carbon nanoribbons

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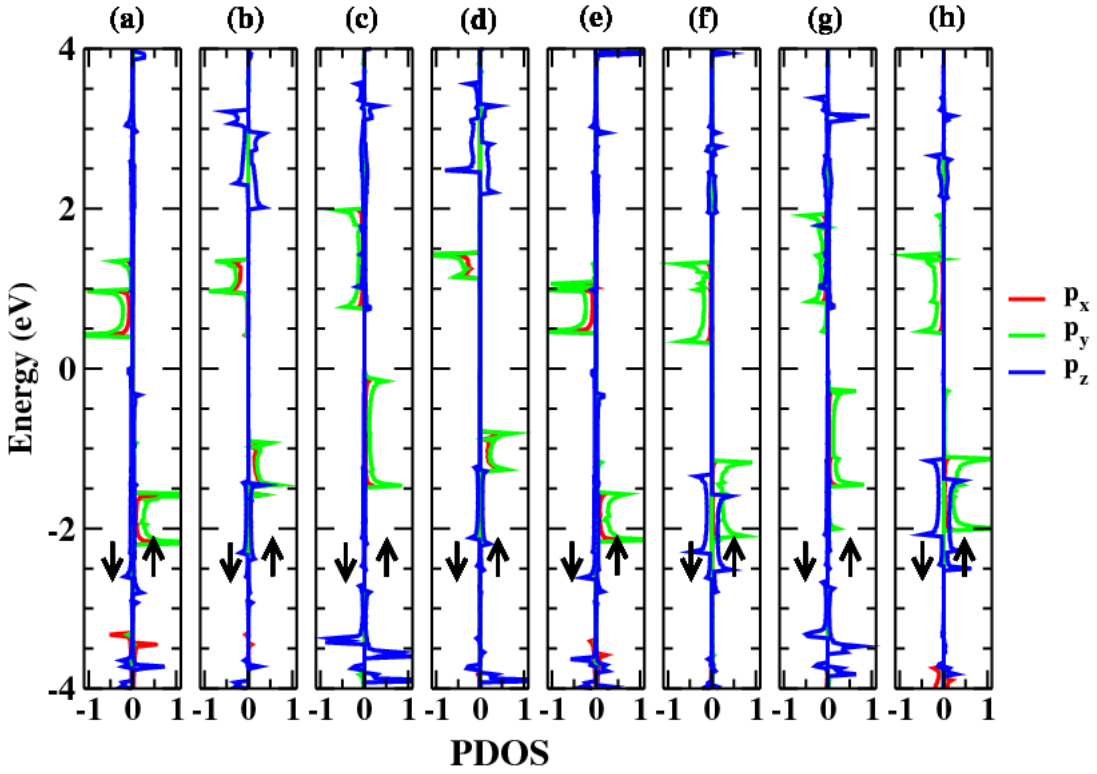

Fig. 1 PDOS of p orbitals of atoms of spin-polarized 6-CC-CC-BNCNRs: (a) upper edge bare C atom of b_3, (b) lower edge bare C atom of b_3, (c) upper edge bare C atom of b_4, (d) lower edge bare C atom of b_4, (e) upper edge bare C atom of b_5, (f) lower edge bare C atom of b_5, (g) upper edge bare C atom of b_6, (h) lower edge bare C atom of b_6. Up and down arrows denote spin-up, and spin-down, states, respectively. Configurations are explained in the main text.

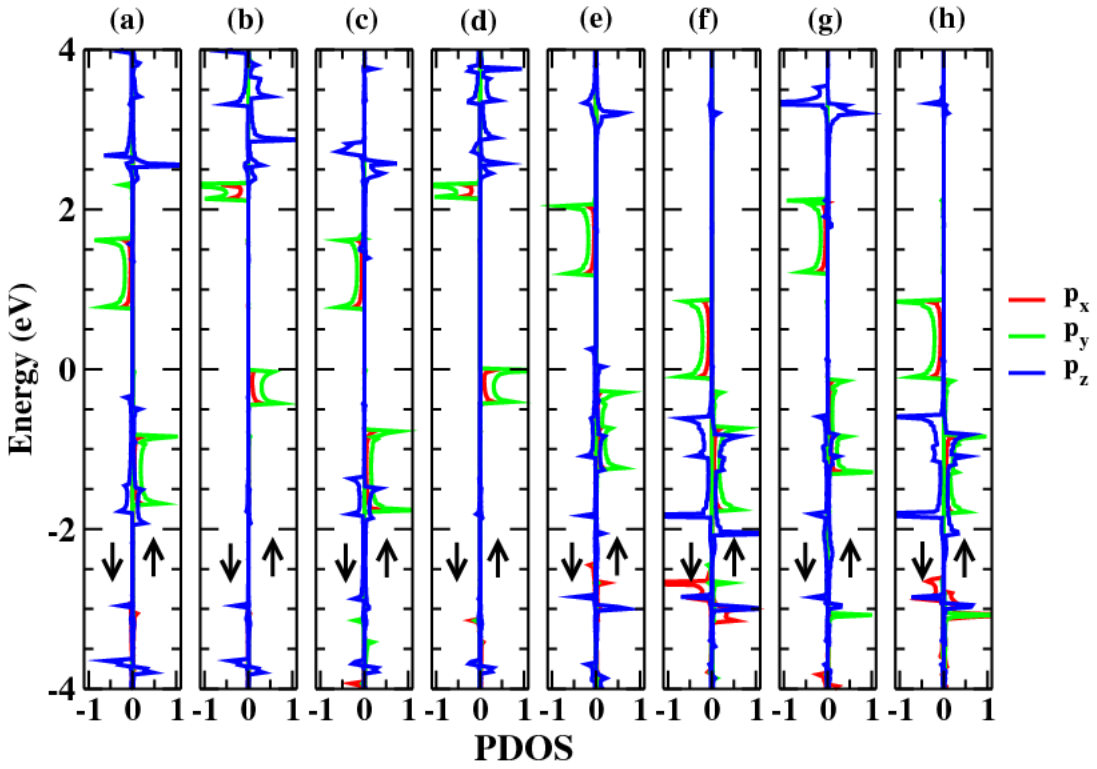

Fig. 2 PDOS of p orbitals of atoms of spin-polarized 6-CC-BN-BNCNRs: (a) upper edge bare C atom of c_3, (b) lower edge bare B atom of c_3, (c) upper edge bare C atom of c_4, (d) lower edge bare B atom of c_4, (e) upper edge bare C atom of c_5, (f) lower edge bare N atom of c_5, (g) upper edge bare C atom of c_6, (h) lower edge bare N atom of c_6. Up and down arrows denote spin-up, and spin-down, states, respectively. Configurations are explained in the main text.

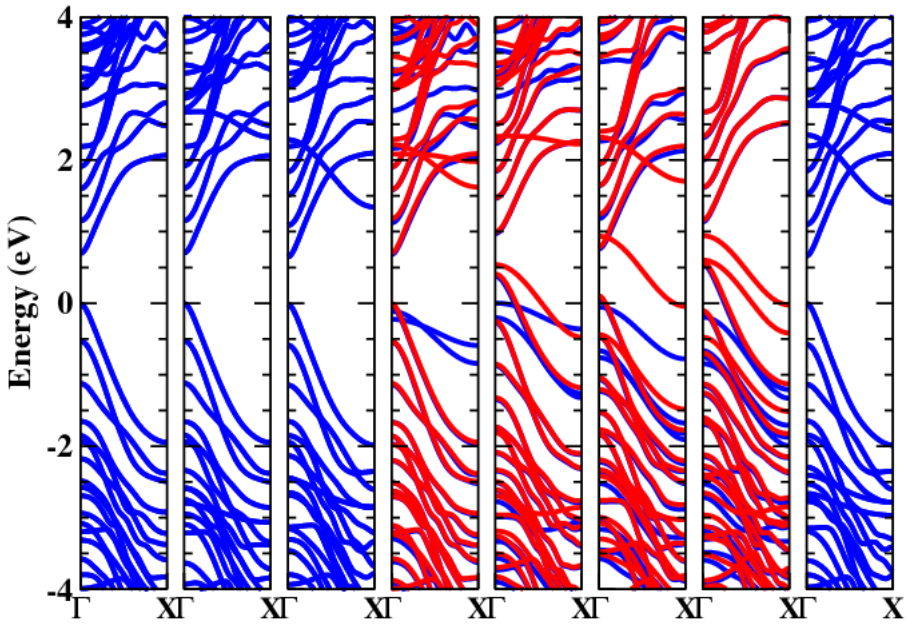

Fig. 3 Band structures of various configurations of 18-BN-BN-ABNCNR: (a) a_0, (b) a_1, (c) a_2, (d) a_3, (e) a_4, (f) a_5, (g) a_6, and (h) a_7. Configurations are explained in the main text.

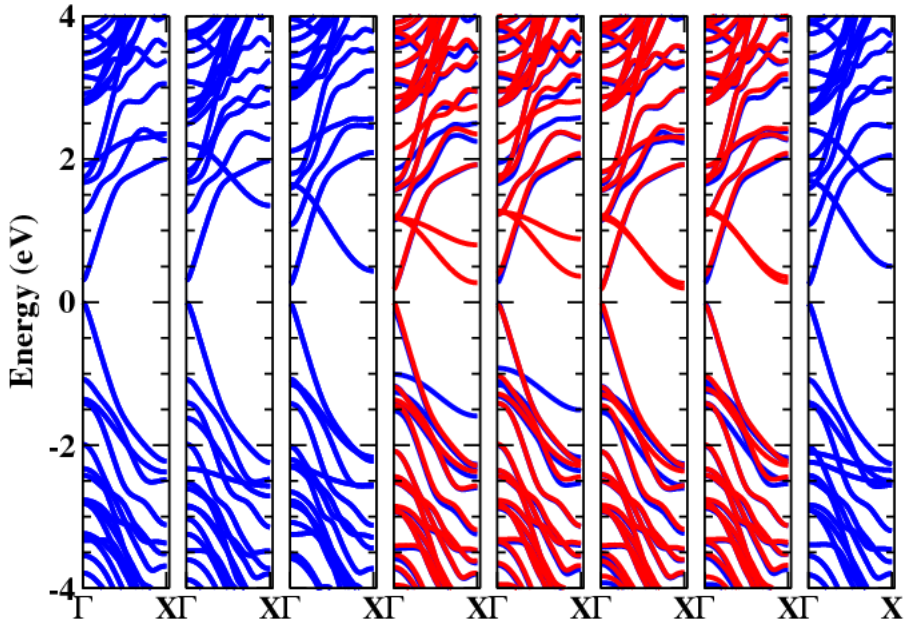

Fig. 4 Band structures of various configurations of 18-CC-CC-ABNCNR: (a) b_0, (b) b_1, (c) b_2, (d) b_3, (e) b_4, (f) b_5, (g) b_6, and (h) b_7. Configurations are explained in the main text.

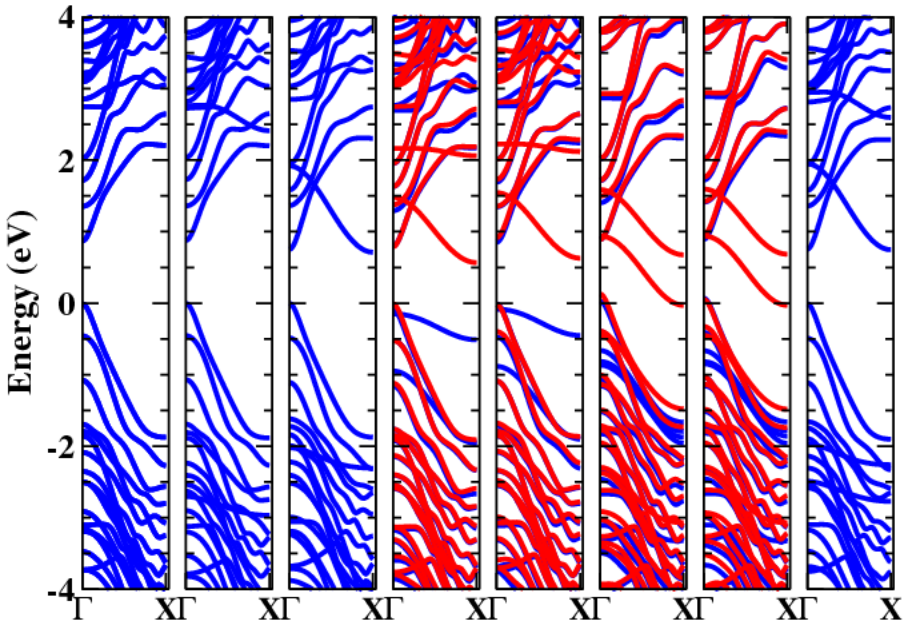

Fig. 5 Band structures of various configurations of 18-CC-BN-ABNCNR: (a) c_0, (b) c_1, (c) c_2, (d) c_3, (e) c_4, (f) c_5, (g) c_6, and (h) c_7. Configurations are explained in the main text.

N_a	Band gaps (eV)							
	b_3		b_4		b_5		b_6	
	Up	Dn	Up	Dn	Up	Dn	Up	Dn
8	1.60	1.07	1.72	1.15	1.73	0.86	1.72	1.05
10	0.86	0.70	0.85	0.59	0.87	0.63	0.92	0.50
12	0.47	0.24	0.38	0.60	0.48	0.23	0.41	0.33
14	1.17	0.74	1.14	0.81	1.17	0.67	1.16	0.71
16	1.02	0.62	0.99	0.72	1.02	0.53	1.01	0.63
18	0.33	0.18	0.27	0.45	0.34	0.19	0.27	0.29

Table 1 Band gaps of CC-CC ABNNCRs for different widths. M denotes the metallic behavior.

N_a	Band gaps (eV)							
	c_3		c_4		c_5		c_6	
	Up	Dn	Up	Dn	Up	Dn	Up	Dn
8	0.50	0.61	M	M	M	M	M	M
10	0.63	0.55	M	M	M	M	M	M
12	0.91	0.94	M	M	M	M	M	M
14	0.31	0.39	M	M	M	M	M	M
16	0.67	0.42	M	M	M	M	M	M
18	0.72	0.71	M	M	M	M	M	M

Table 2 Band gaps of BN-BN ABNNCRs for different widths. M denotes the metallic behavior.