Electronic supplementary information

Realizing the Diverse Electronic and Magnetic Properties in the Hybrid Zigzag BNC Nanoribbons via Hydrogenation

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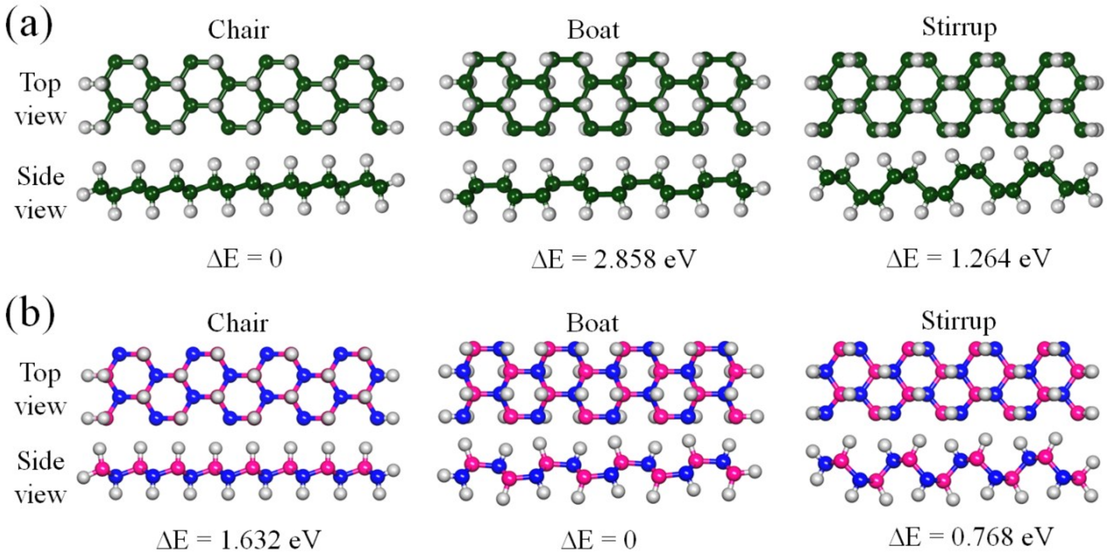


Figure S1. Top and side views of *f*H-zGNR (a) and *f*H-zBNNR (b) with chair, boat and stirrup configurations, as well asthe relative energies (ΔE) of different configurations to the most one. It is shown that the chair-like and boat-like configurations are the energetically most favorable for *f*H-zGNR and *f*H-zBNNR, respectively.

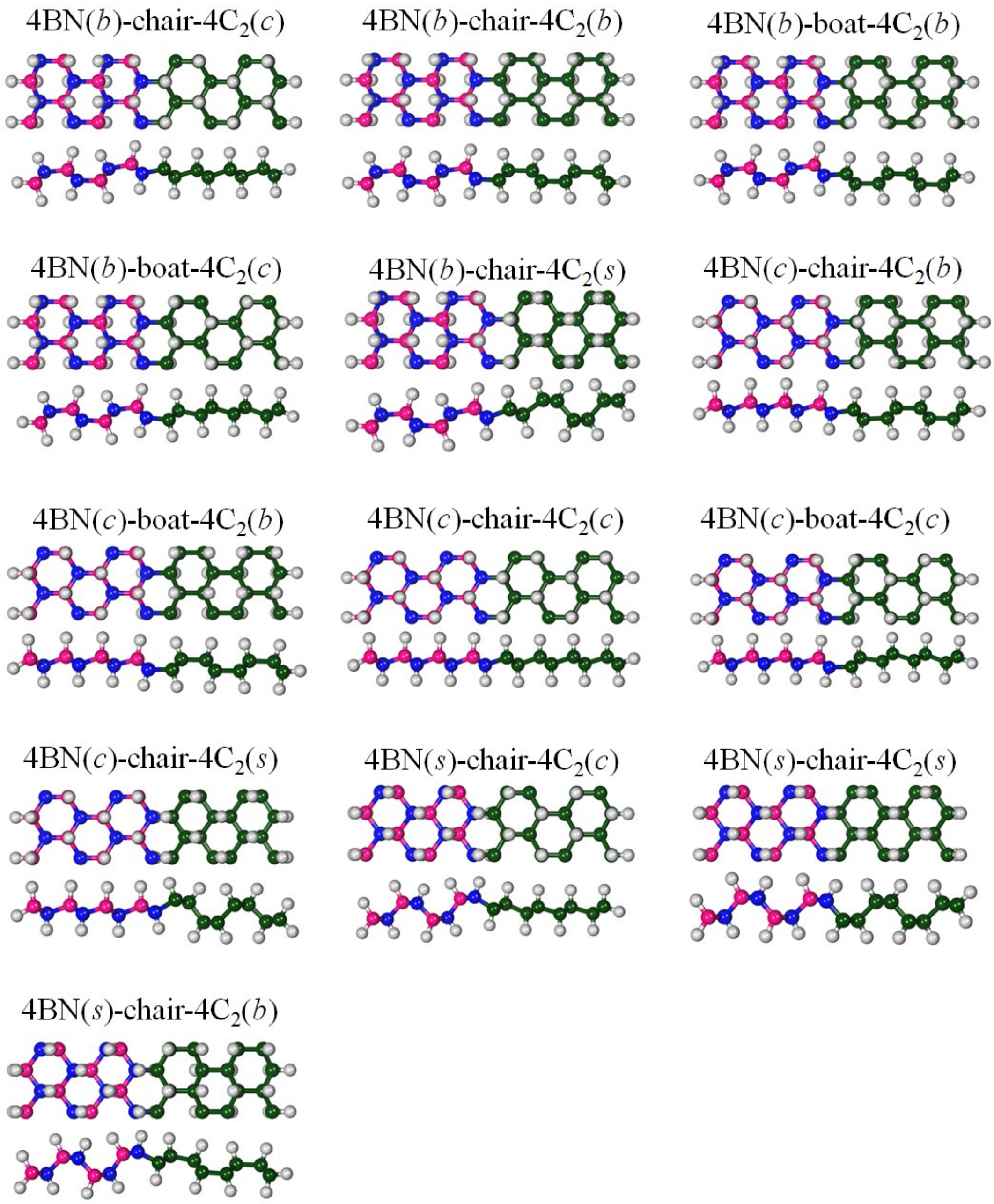


Figure S2. The obtained geometrical structures of the fully hydrogenated *f*H-zBNCNRs with the interfacial N-C connectionby considering three possible hydrogenated configurations of chair, boat and stirrup for the constituent BN or C segment, as well as two possible modes of connection (chair or boat) between these two segments.

Table S1. The relative energies (ΔE) of different magnetic couplings to the ground state and the corresponding electronic properties for the possible *f*H-zBNCNR configurations with the interfacial N-C connection, as well as their relative energies (E_{rel}) to the lowest-lying one. NM, FM and AFM represent the nonmagnetic, ferromagnetic and antiferromagnetic spin couplings, respectively.

System	E_{rel} (meV)	ΔE (meV)			Electronic properties	Band gap (eV)
		NM	FM	AFM		
4BN(*b*)-chair-4C_2(*c*)	0.0	0.0	--	--	Semiconductor	1.756
4BN(*b*)-chair-4C_2(*b*)	1160.2	0.0	--	--	Semiconductor	1.703
4BN(*b*)-boat-4C_2(*b*)	1592.3	0.0	--	--	Semiconductor	1.721
4BN(*b*)-boat-4C_2(*c*)	359.7	0.0	--	--	Semiconductor	1.756
4BN(*b*)-chair-4C_2(*s*)	769.8	0.0	--	--	Semiconductor	1.547
4BN(*c*)-chair-4C_2(*b*)	2350.3	1.9	0.0	1.6	Metallicity	--
4BN(*c*)-boat-4C_2(*b*)	2796.6	1.1	0.0	0.3	Metallicity/Half-metallicity	--
4BN(*c*)-chair-4C_2(*c*)	1123.8	0.0	4.6	13.7	Semiconductor	0.020
4BN(*c*)-boat-4C_2(*c*)	1633.4	2.1	0.0	2.3	Half-metallicity	--
4BN(*c*)-chair-4C_2(*s*)	1922.2	1.7	1.8	0.0	Half-metallicity	--
4BN(*s*)-chair-4C_2(*c*)	414.5	4.0	0.0	3.0	Metallicity	--
4BN(*s*)-chair-4C_2(*s*)	1826.7	4.8	0.9	0.0	Metallicity/Half-metallicity	--
4BN(*s*)-chair-4C_2(*b*)	2867.9	4.5	0.1	0.0	Metallicity/Half-metallicity	--

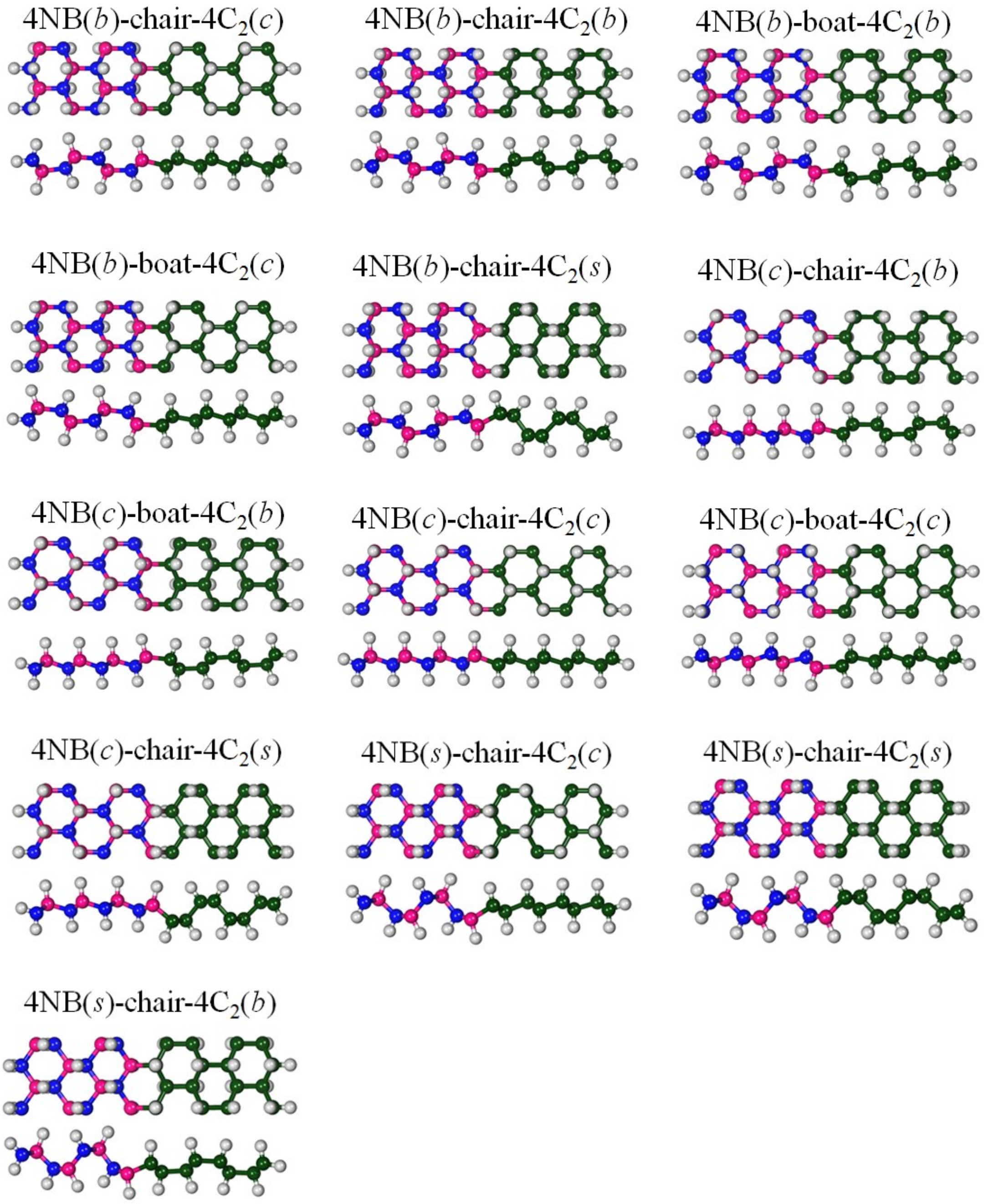


Figure S3. The obtained geometrical structures of the fully hydrogenated *f*H-zBNCNRs with the interfacial B-C connectionby considering three possible hydrogenated configurations of chair, boat and stirrup for the constituent BN or C segment, as well as two possible modes of connection (chair or boat) between these two segments.

Table S2. The relative energies (ΔE) of different magnetic couplings to the ground state and the corresponding electronic properties for the possible *f*H-zBNCNR configurations with the interfacial B-C connection, as well as their relative energies (E_{rel}) to the lowest-lying one. NM, FM and AFM represent the nonmagnetic, ferromagnetic and antiferromagnetic spin couplings, respectively.

System	**E_{rel} (meV)**	**ΔE (meV)**			**Electronic properties**	**Band gap (eV)**
		NM	**FM**	**AFM**		
4NB(*b*)-chair-4C_2(*c*)	0.0	0.0	--	--	Semiconductor	0.217
4NB(*b*)-chair-4C_2(*b*)	1180.4	0.0	--	--	Semiconductor	0.328
4NB(*b*)-boat-4C_2(*b*)	1376.9	0.0	--	--	Semiconductor	0.466
4NB(*b*)-boat-4C_2(*c*)	199.9	0.0	--	--	Semiconductor	0.479
4NB(*b*)-chair-4C_2(*s*)	945.0	0.0	--	--	Semiconductor	0.289
4NB(*c*)-chair-4C_2(*b*)	2355.9	5.7	0.0	0.3	Metallicity/Half-metallicity	--
4NB(*c*)-boat-4C_2(*b*)	2754.9	6.1	0.0	0.1	Metallicity/Half-metallicity	--
4NB(*c*)-chair-4C_2(*c*)	922.4	6.4	1.4	0.0	Half-metallicity	--
4NB(*c*)-boat-4C_2(*c*)	1545.5	6.4	1.8	0.0	Half-metallicity	--
4NB(*c*)-chair-4C_2(*s*)	1575.2	3.8	0.2	0.0	Metallicity/Half-metallicity	--
4NB(*s*)-chair-4C_2(*c*)	1112.3	4.2	0.9	0.0	Metallicity/Half-metallicity	--
4NB(*s*)-chair-4C_2(*s*)	1661.8	9.4	0.9	0.0	Metallicity/Half-metallicity	--
4NB(*s*)-chair-4C_2(*b*)	2753.7	9.0	2.4	0.0	Half-metallicity	--

Table S3. The most favorable boat conformation and the corresponidng nonmagentic (NM) ground state for the fully hydrogenated *f*H-4-zBNNR and *f*H-6-zBNNR systems.

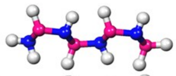
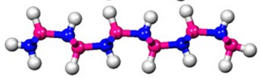
System		ΔE (meV)		
		NM	FM	AFM
*f*H-4-zBNNR		0.0	--	--
*f*H-6-zBNNR		0.0	--	--

Table S4. Total magnatic moment per supercell for the magnetic ground states of *f*H-8-zBNNR, as well as fully and partially hybrid hydrogenated zBNCNRs systems. FM and AFM represent the ferromagnetic and antiferromagnetic spin couplings, respectively.

Conformation	Ground State	Total Magnetic Moment(μB)
*f*H-8-zBNNR	FM/AFM	0.206/0.000
6NB(*b*)-chair-2C_2(*c*)	AFM	0.000
8BN(*b*)-chair-8C_2(*c*)	FM	0.256
10BN(*b*)-chair-10C_2(*c*)	AFM	0.000
6NB(*b*)-chair-6C_2(*c*)	FM	0.259
8NB(*b*)-chair-8C_2(*c*)	FM	0.466
10NB(*b*)-chair-10C_2(*c*)	AFM	0.168
*p*H-$(BN)_4(C_2)_4$- *II*(2,0)	AFM	0.000
*p*H-$(BN)_4(C_2)_4$- *II*(4,0)	AFM	0.000
*p*H-$(BN)_4(C_2)_4$- *II*(4,2)	AFM	0.130
*p*H-$(NB)_4(C_2)_4$- *II*(2,0)	AFM	0.000
*p*H-$(NB)_4(C_2)_4$- *II*(4,0)	AFM	0.208
*p*H-$(NB)_4(C_2)_4$- *II*(4,2)	AFM	0.084
*p*H-$(BN)_4(C_2)_4$-*III*(1,1)	AFM	0.000
*p*H-$(NB)_4(C_2)_4$-*III*(1,1)	AFM	0.000

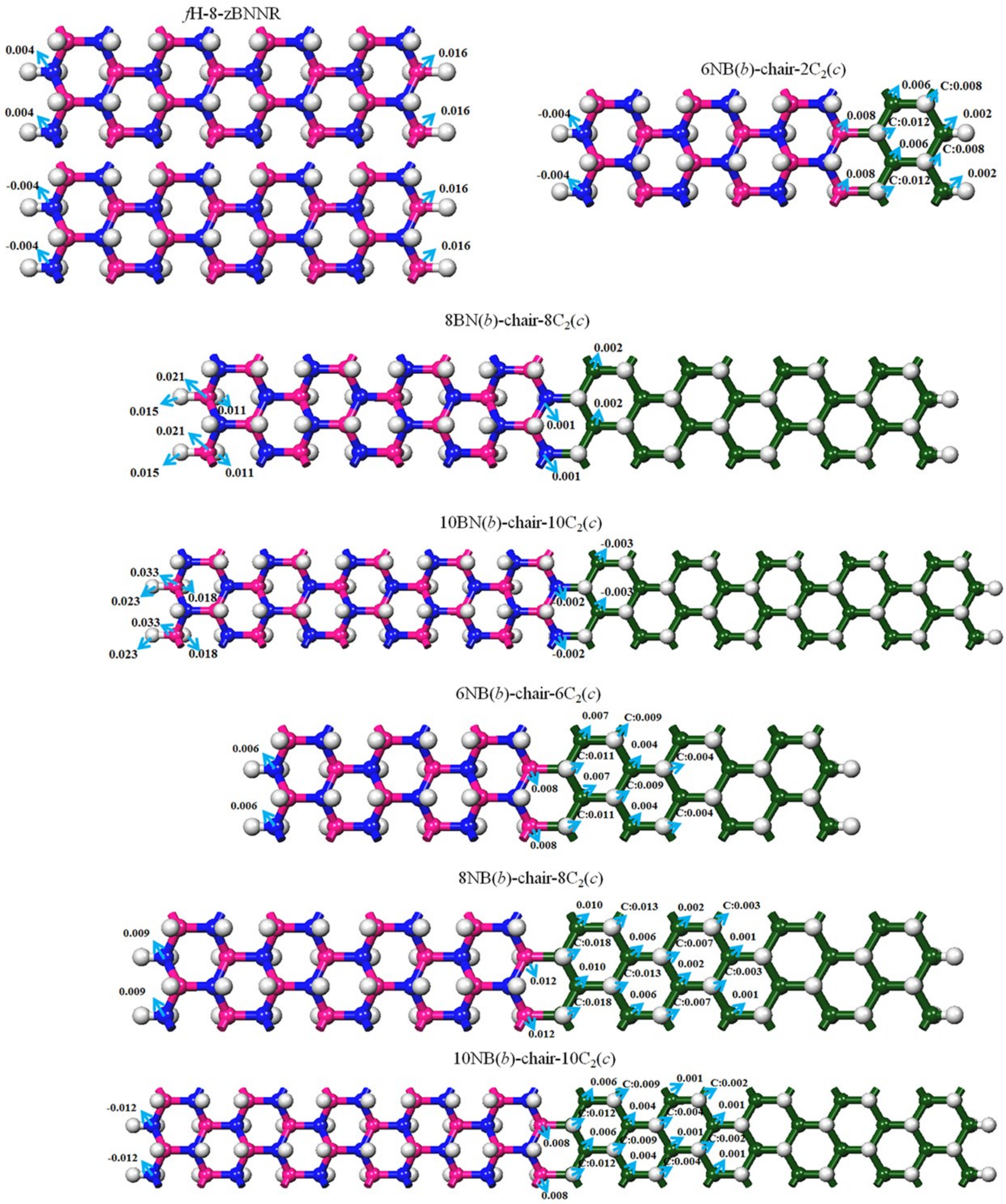


Figure S4. The distribution of atomic magnetic moments M (μB) in supercell for the magnetic ground states of *f*H-8-zBNNR and fully hydrogenated zBNCNRs systems.

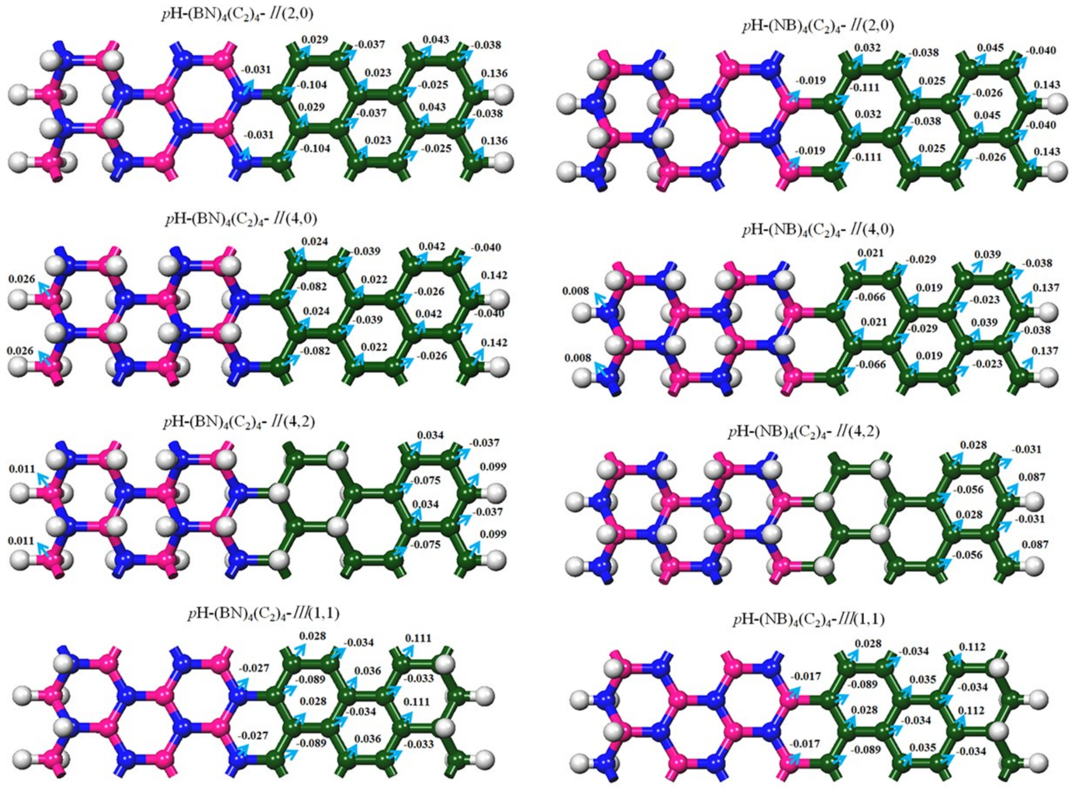


Figure S5. The distribution of atomic magnetic moments M (μB) in supercell for the magnetic ground states of partially hydrogenated zBNCNRs systems.