Supporting Information for:

Ferromagnetic Dirac half-metallicity in edge-modified zigzag boron nitride nanoribbons

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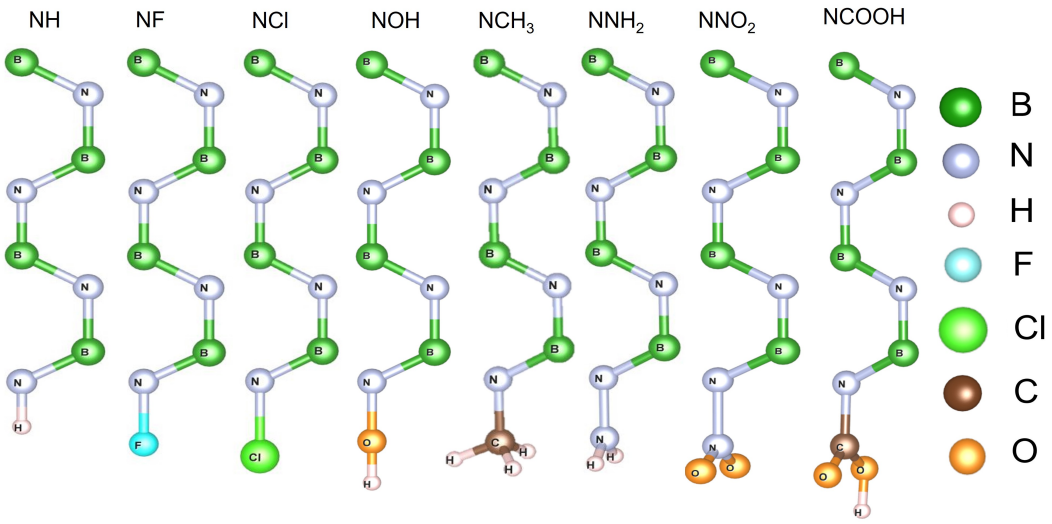

Figure S1: Geometry of ZBNNRs-NX (shown here with n = 2) with functional groups (X): H, F, Cl, OH, CH_3, NH_2, NO_2, and COOH. CH_3, NH_2, and COOH.

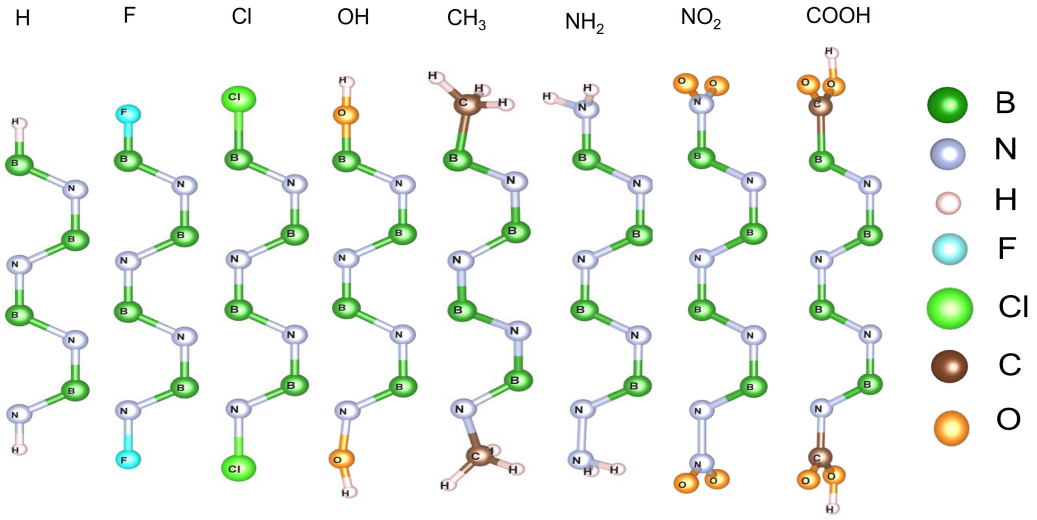

Figure S2: Geometry of ZBNNRs-BX-NX (here with n = 2). Both edges are passivated with functional groups (X): H, F, Cl, OH, CH_3, NH_2, NO_2, and COOH. CH_3, NH_2, and COOH.

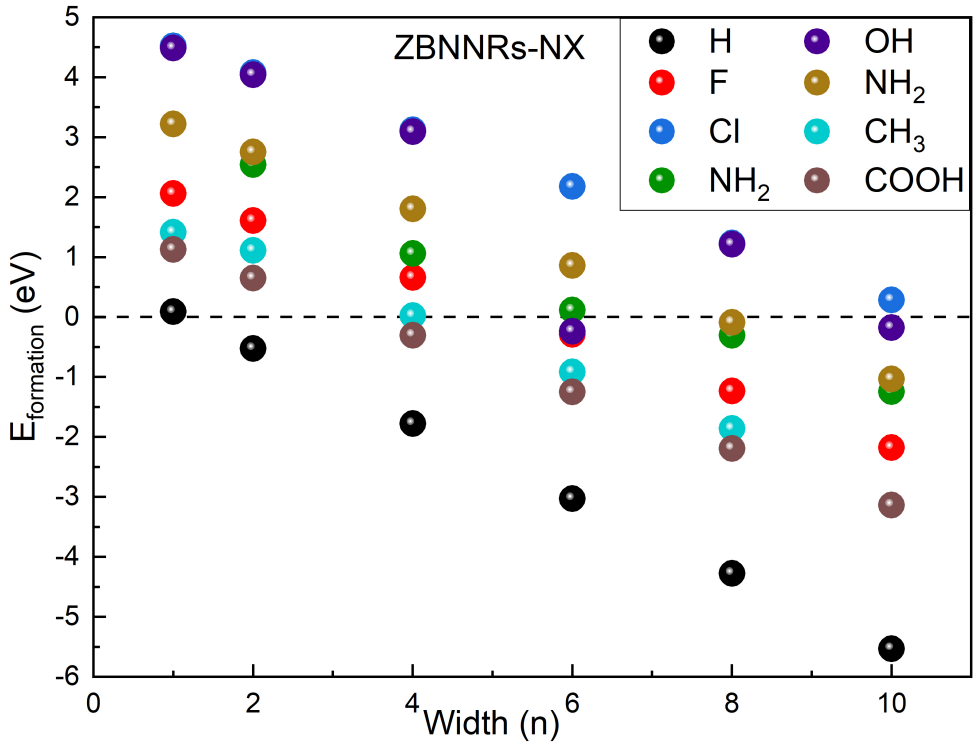

Figure S3: The formation energy $E_{formation}$ with respect to thickness (n) of ZBNNRs-NX.

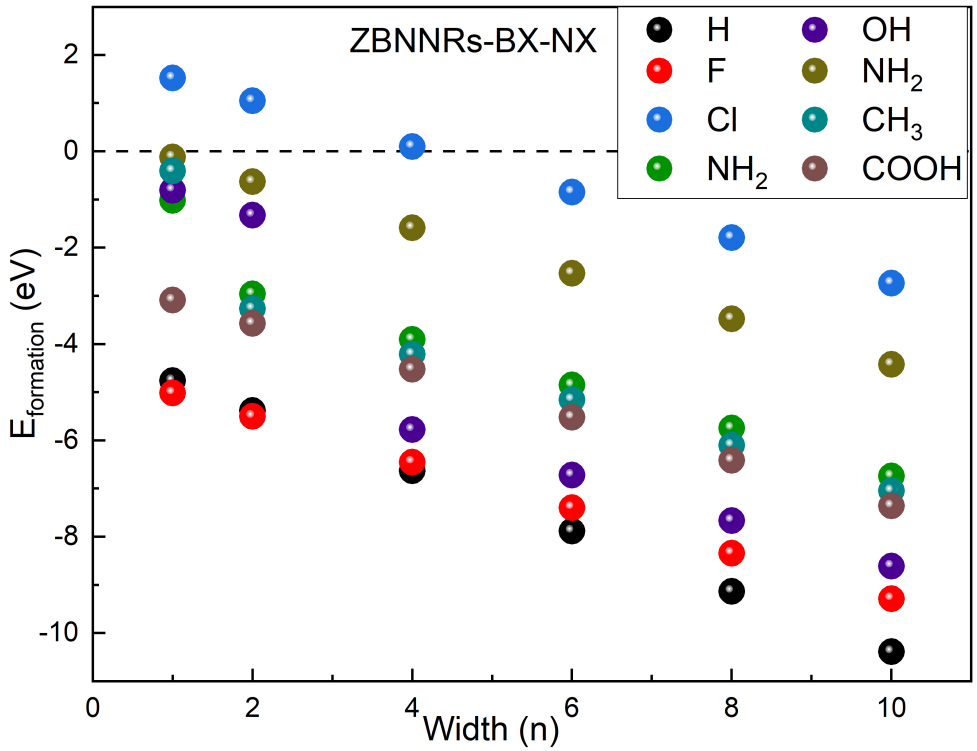

Figure S4: The formation energy $E_{formation}$ with respect to thickness (n) of ZBNNRs-BX-NX.

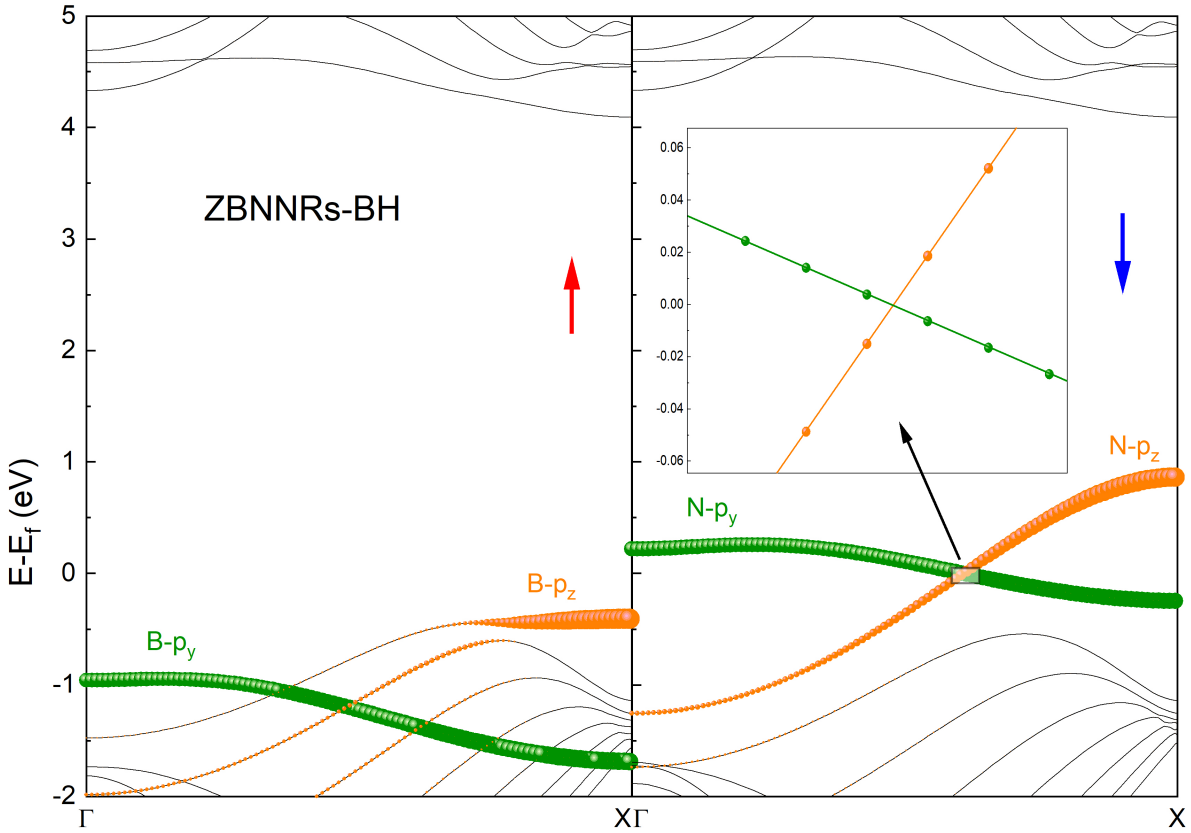

Figure S5: Spin polarized projected band structure for ZBNNRs-BH (n = 3). Size of ball shows the contribution of orbitals

Table S1: The spin polarized energy gap, the total energy difference with and without SOC effects E_{diff} = $E_{DFT+SOC}$ - E_{DFT}, energy difference △E between FM and AFM configuration, and magnetic exchange coupling parameters J_0 for ZBNNRs-BX with width n = 3.

Spin resolved band gap (eV)									
n	Spin	H	F	OH	COOH	CH_3	Cl	NH_2	NO_2
1	up	4.385	5.137	3.679	3.073	metal	0.400	metal	1.833
	dn	0.099	0.114	0.017	0.050	metal	metal	metal	0.011
2	up	4.377	4.836	3.542	2.892	3.084	1.756	1.543	1.675
	dn	0.032	0.095	0.127	0.008	metal	metal	metal	0.048
4	up	4.505	4.759	3.545	2.863	2.766	1.393	1.118	1.964
	dn	0.018	0.085	0.085	0.038	metal	metal	metal	0.024
6	up	4.580	4.734	3.549	3.521	2.883	1.301	0.925	1.629
	dn	0.020	0.086	0.076	0.062	0.031	metal	metal	0.005
8	up	4.562	4.657	3.571	2.887	2.752	1.164	metal	1.619
	dn	0.026	0.086	0.075	0.036	0.026	metal	metal	0.066
10	up	4.536	4.535	3.548	3.491	2.742	1.085	0.890	1.620
	dn	0.131	0.058	0.071	0.059	0.031	metal	0.030	0.016
SOC effect on total energy (meV)									
E_{diff}		-0.6	-0.8	-0.7	-0.81	-0.7	-0.2	-0.8	-0.9
△E (eV) = E_{AFM} - E_{FM}									
△E		0.138	0.166	0.115	0.117	0.115	0.173	0.129	0.248
Nearest magnetic exchange parameter J_0 (eV)									
J_0(eV)		0.138	0.166	0.115	0.117	0.115	0.173	0.129	0.248

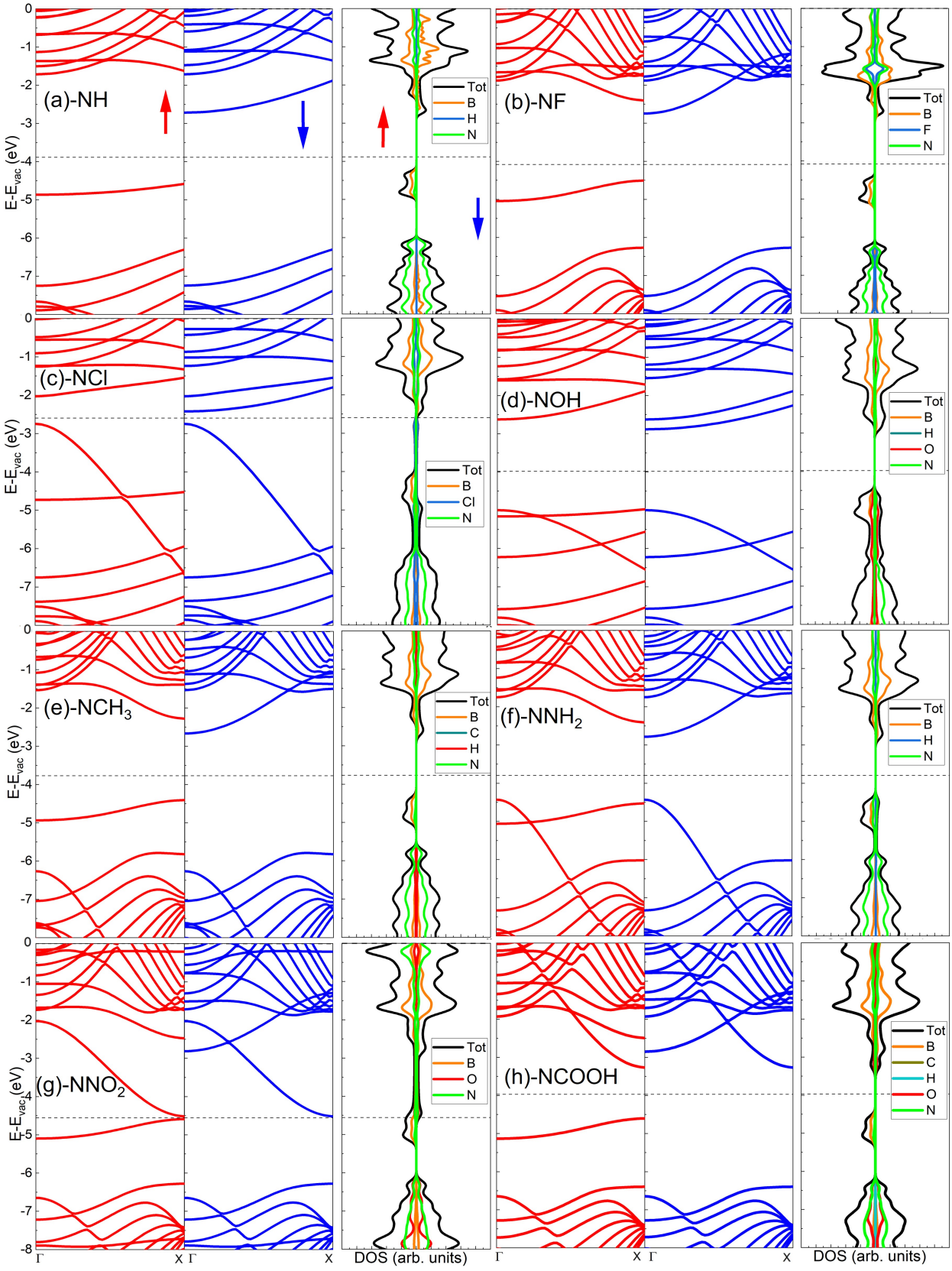

Figure S6: Majority spin (red), minority spin (blue), density of states for ZBNNRs-NX where X = (a) H, (b) F, (c) Cl, (d) OH, (e) CH_3, (f) NH_2, (g) NO_2 (h) COOH. All NRs have energy gap in semiconducting range for spins except X = NO_2, which behaves as half metal.

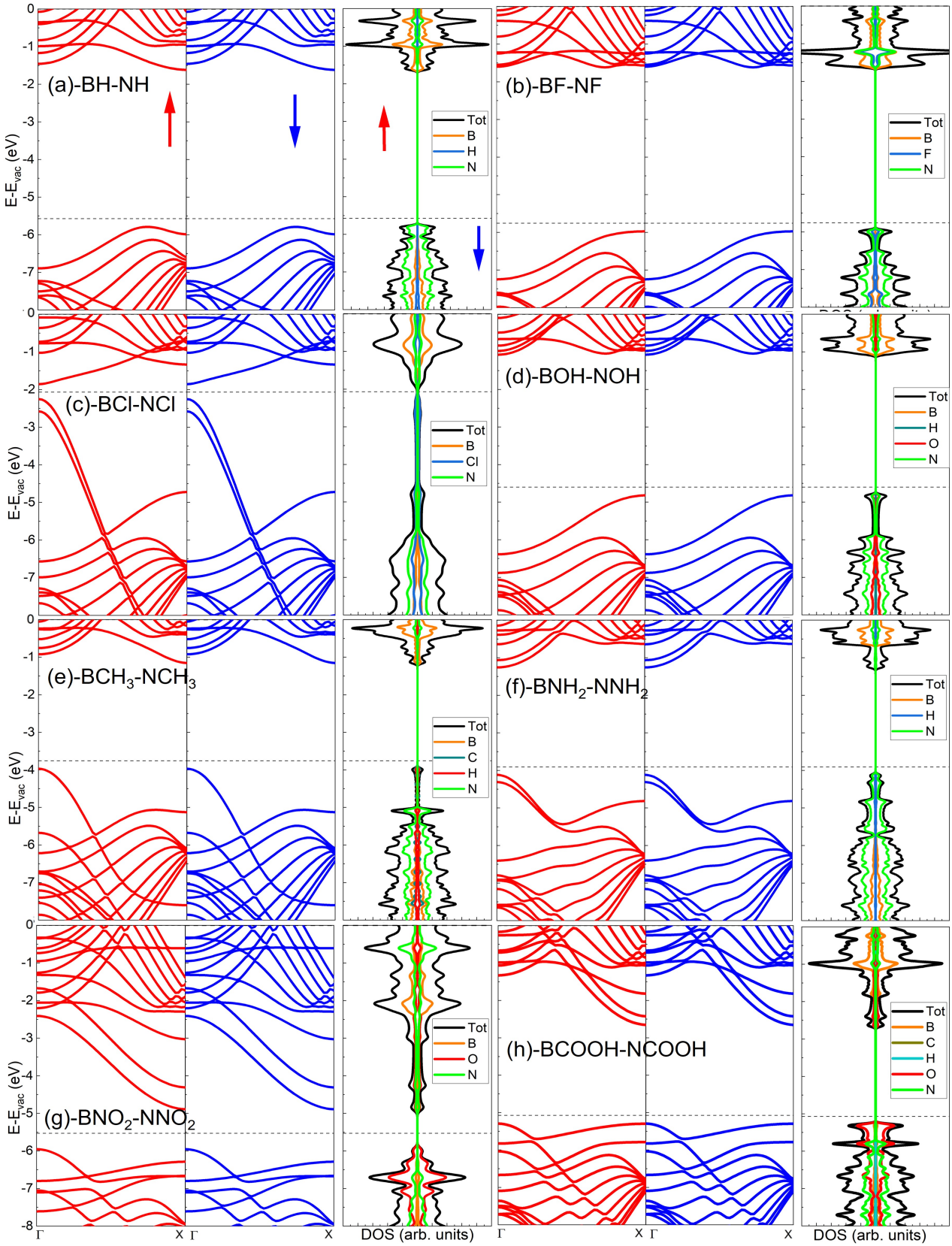

Figure S7: Band structure for Majority spin (red), minority spin (blue), and density of states for ZBNNRs-BX-NX, where X = (a) H, (b) F, (c) Cl, (d) OH, (e) CH_3, (f) NH_2, (g) NO_2, and (h) COOH.

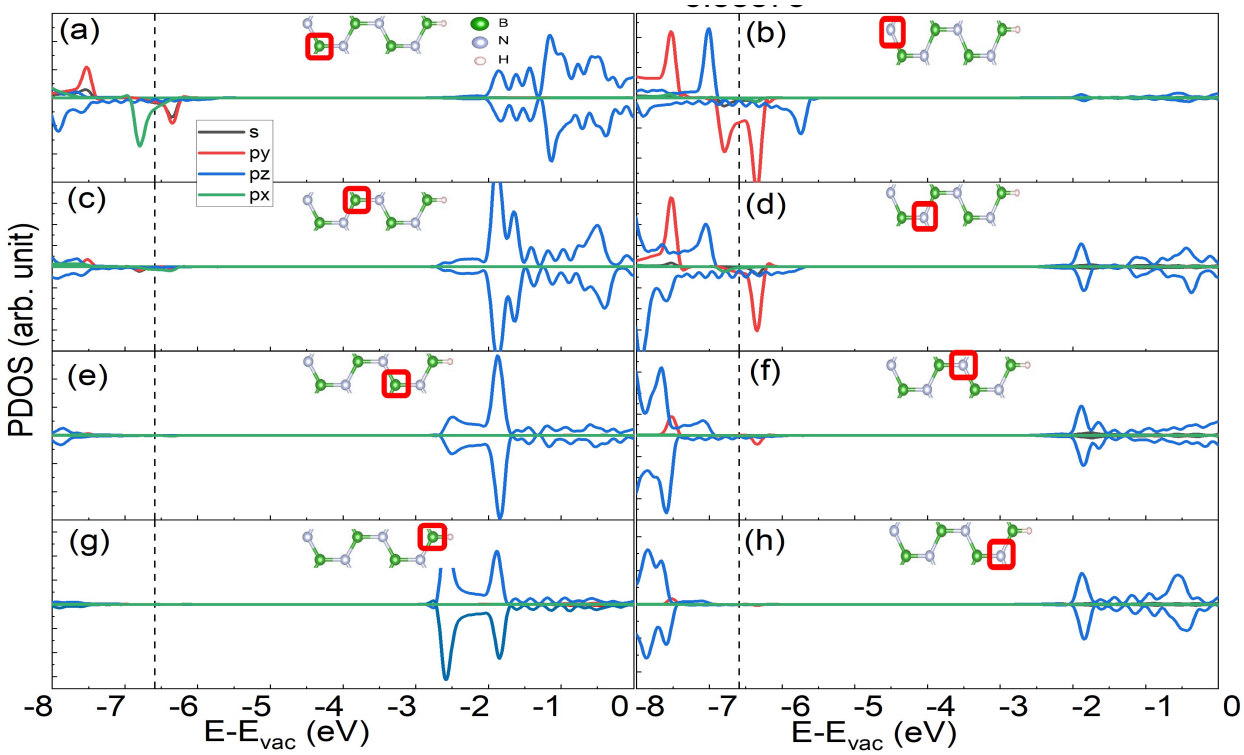

Figure S8: Projected density of states of each boron atom in (a, c, e, g) and nitrogen atom (specified by red boxes) in (b, d, f, h) for ZBNNRs-BH with n = 2.

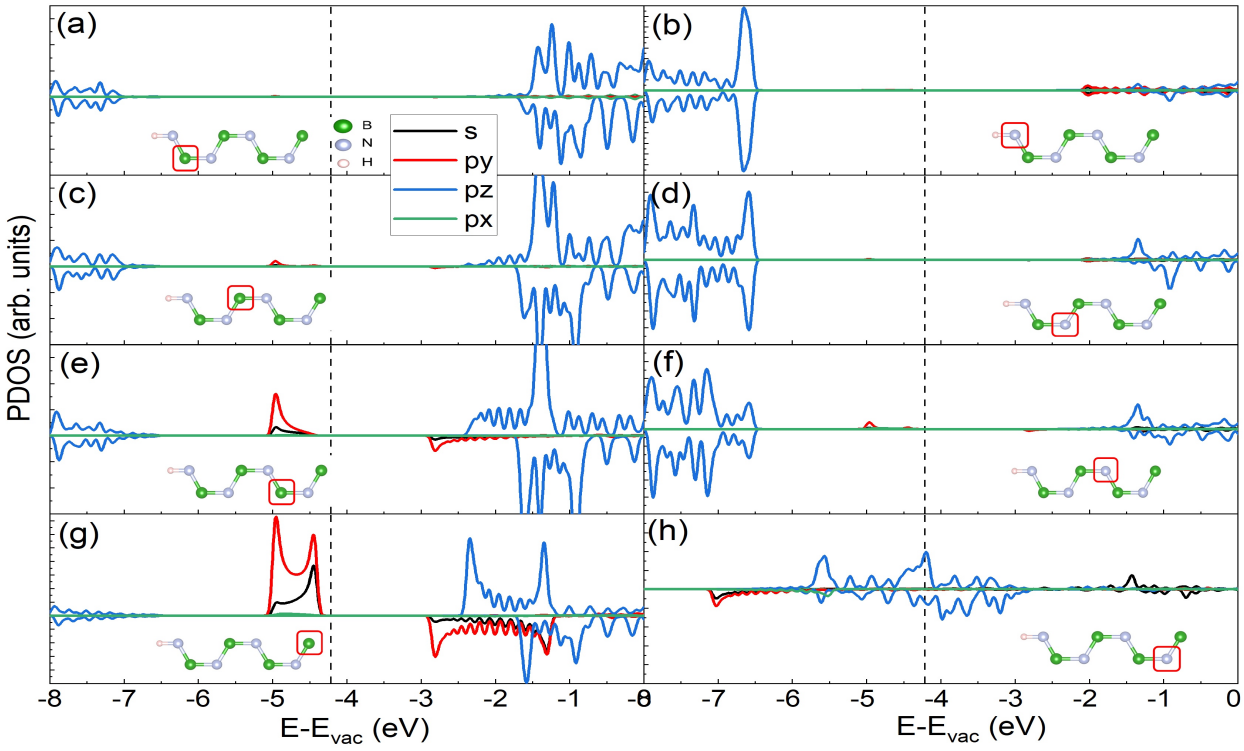

Figure S9: Projected density of states of each boron atom in (a, c, e, g) and nitrogen atom (specified by red boxes) in (b, d, f, h) for ZBNNRs-NH with n = 2.

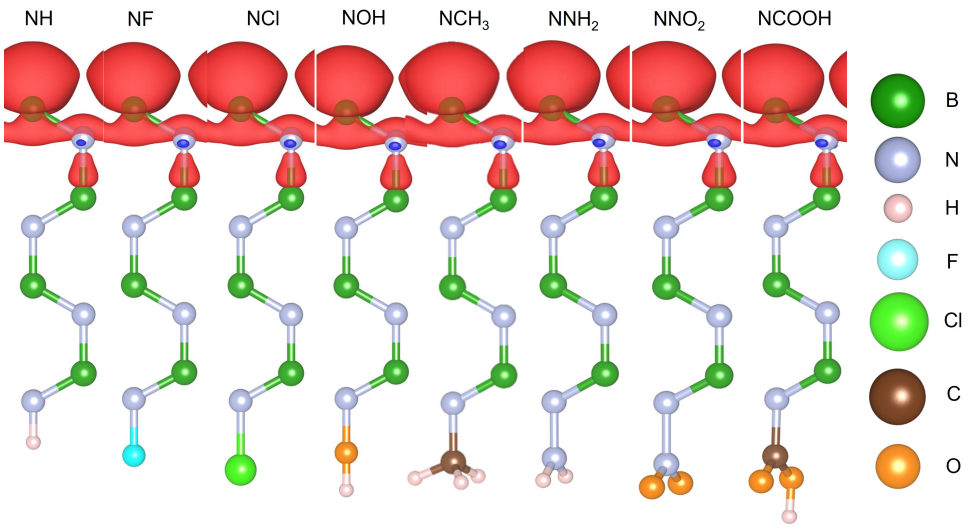

Figure S10: Electron spin density of ZBNNRs-NX (with n = 2) with X = H, F, Cl, OH, CH_3, NH_2, NO_2, and COOH. Red and blue color show spin-up and spin-down density with an isosurface value of 0.005 $Bohr^{-3}$.

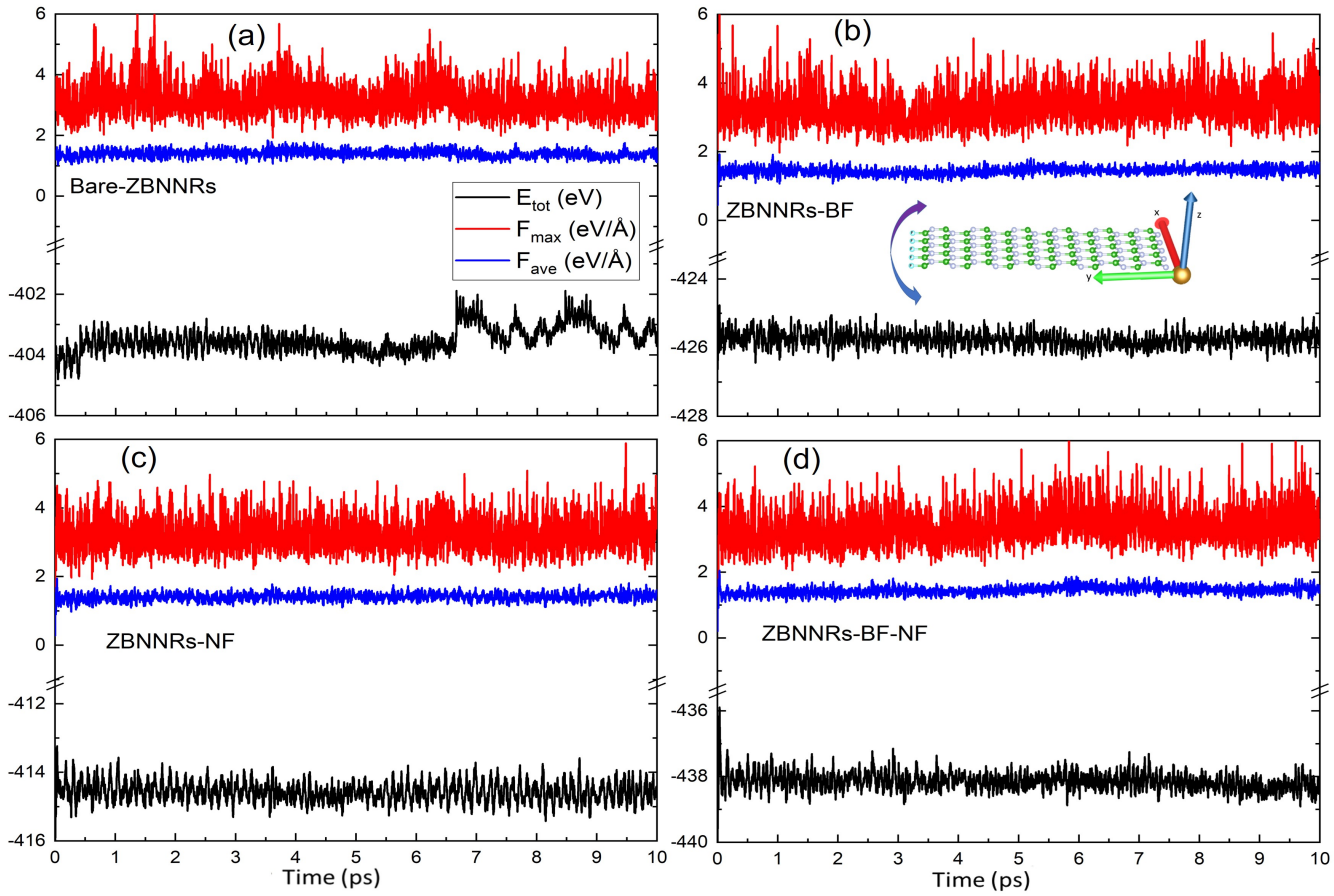

Figure S11: Evolution of total energy, maximum and average forces with respect to time for (a) bare, (b-d) ZBNNRs-BF, (c) ZBNNRs-NF, and (d) ZBNNRs-BF-NF.

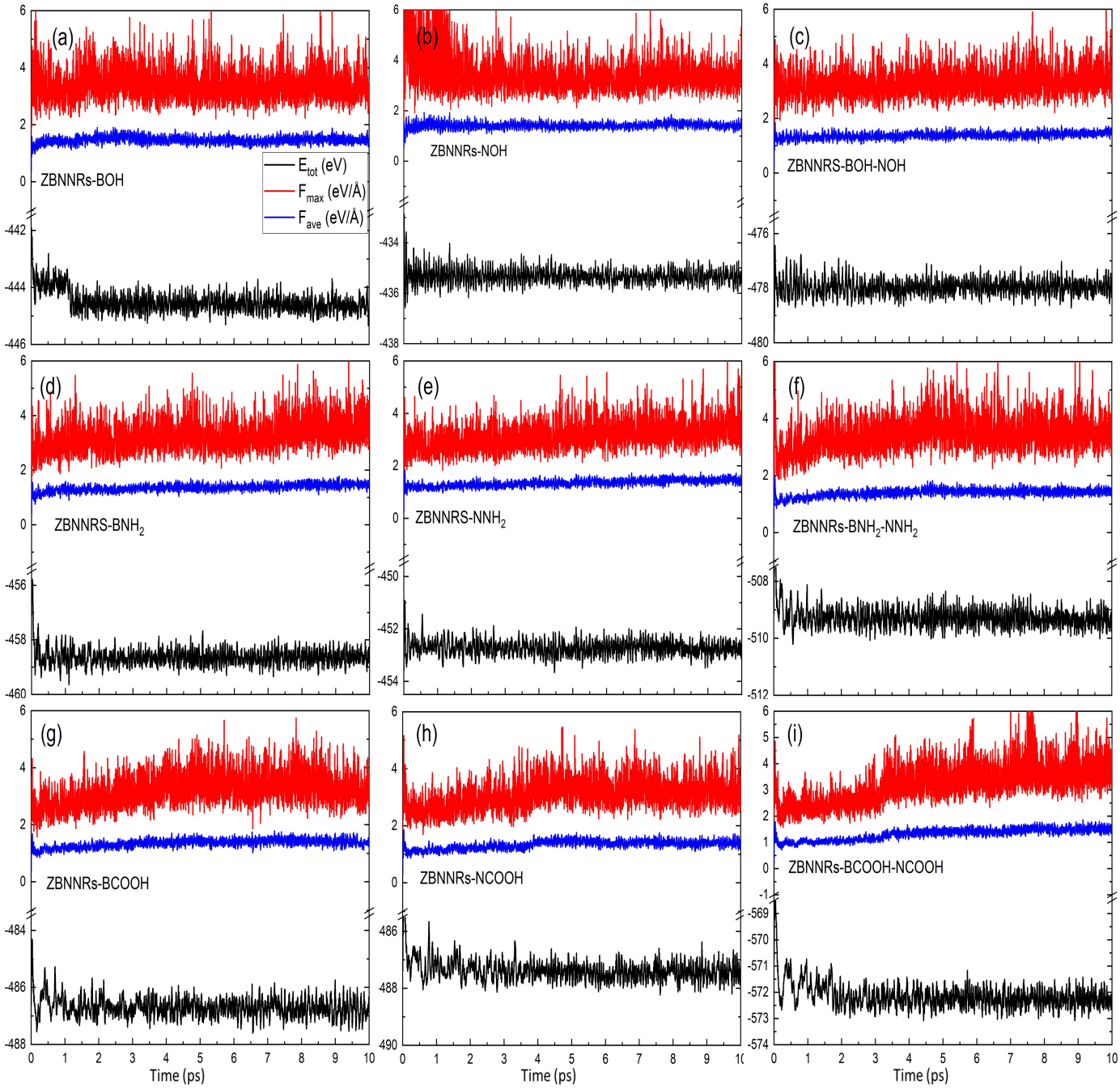

Figure S12: Evolution of total energy, maximum and average forces with respect to time for ZBNNRs with (a-c) OH, (d-f) NH_2, and (g-i) COOH.

Table S2: Spin polarized energy gap (eV) of ZBNNRs-NX with respect to width (n).

n	Spin	H	F	OH	COOH	CH_3	Cl	NH_2	NO_2
1	up	2.097	2.241	1.743	1.296	2.123	0.689	1.423	0.116
	dn	3.84	3.074	1.717	3.166	3.666	0.074	2.660	1.853
2	up	2.058	2.112	1.685	1.254	2.1394	0.721	0.577	0.064
	dn	3.723	3.511	2.009	3.139	2.704	0.406	0.067	1.780
4	up	2.053	2.111	2.006	1.343	2.1329	0.713	2.029	0.075
	dn	3.401	3.525	1.760	3.136	3.122	0.323	1.649	1.764
6	up	2.053	2.111	2.123	1.358	2.1311	0.623	1.871	0.083
	dn	3.172	3.528	2.460	3.134	2.868	0.236	1.491	1.761
8	up	2.047	2.113	1.711	1.534	2.1265	0.595	0.511	0.077
	dn	3.19	3.536	1.308	3.136	2.734	0.208	0.052	1.757
10	up	2.051	2.113	2.222	1.593	1.0173	0.587	0.477	0.083
	dn	2.889	3.537	1.682	3.136	1.017	0.211	0.055	1.756

Table S3: Spin polarized energy gap (eV) of ZBNNRs-BX-NX with respect to width (n).

n	Spin	H	F	OH	COOH	CH_3	Cl	NH_2	NO_2
1	up	4.548	4.349	1.746	2.466	2.770	0.319	0.025	0.782
	dn	4.548	4.349	1.746	2.466	2.768	0.319	0.186	0.782
2	up	4.423	4.393	1.695	2.579	2.817	0.335	2.863	0.894
	dn	4.423	4.393	1.695	2.579	2.817	0.335	2.864	0.894
4	up	4.176	4.366	3.747	2.645	2.819	0.398	2.859	1.066
	dn	4.176	4.366	3.746	2.645	2.819	0.398	2.859	1.066
6	up	3.992	4.326	3.711	0.794	2.806	0.468	2.861	1.150
	dn	3.992	4.326	3.710	0.016	2.806	0.468	2.861	1.150
8	up	4.010	4.295	3.700	2.818	2.814	0.501	2.816	1.316
	dn	4.010	4.298	3.708	2.818	2.814	0.500	2.808	1.316
10	up	3.771	4.282	3.696	2.843	2.808	0.502	2.891	1.350
	dn	3.771	4.288	3.701	2.843	2.808	0.501	2.888	1.350