Electronic Supplementary Information

Tunable the electronic structure and magnetic moment of the C_2N nanoribbons with different edge functionalization atoms

Yusheng Wang[1,3*], Nahong Song[2,3], Min Jia[1], Dapeng Yang[1], Yuye Yang[2], Chikowore Panashe[a], Jianjun Wang[4]

1) College of Mathematics and Information Science, North China University of Water Resources and Electric Power, Zhengzhou, Henan, 450011, China

2) College of computer and information engineering, and university of economics and law, Zhengzhou, Henan, 450000, China

3) International Joint Research Laboratory for Quantum Functional Materials of Henan, and School of Physics and Engineering, Zhengzhou University, Zhengzhou 450001, China

4) College of Science, Zhongyuan University of Technology, Zhengzhou 450007, China

Table S1. The lattice constants (Å), the C–C–N bond angle (α), the C–N–C bond angle(β), the C–C–C bond angle(γ), bond length (Å)in pristine and saturated systems

	Z-C_2NNR						A1-C_2NNR	A2-C_2NNR
system	b	α(deg)	β(deg)	γ(deg)	d_{C-N}	d_{C-C}	a_1	a_2
sheet	14.428	118.836	117.620	119.980	1.336	1.469	8.330	8.330
pristine	14.470	137.20	163.110	123.100	1.238	1.382	8.359	8.364
H	14.428	120.67	120.980	120.410	1.321	1.443	8.332	8.333
O	14.420	113.400	111.763	114.466	1.359	1.527	8.340	8.343
F	14.437	124.24	126.780	123.620	1.304	1.449	8.334	8.334
OH	14.429	115.055	112.376	118.630	1.346	1.530	8.338	8.336
OF	14.438	116.087	109.822	122.888	1.344	1.517	8.339	8.334

Table S2. The different direction diameter (d_1, d_2, d_3) of the inscribed circle formed by the nitride atoms in pristine and saturated systems for a series of ribbon widths

Width	C_2NNR	Z-C_2NNR			A1-C_2NNR			A2-C_2NNR		
		d_1(Å)	d_2(Å)	d_3(Å)	d_1(Å)	d_2(Å)	d_3(Å)	d_1(Å)	d_2(Å)	d_3(Å)
1	Pristine	6.636	5.576	5.689	5.568	5.540	5.542	5.585	5.615	5.611
	H	5.545	5.491	5.496	5.519	5.497	5.494	5.519	5.516	5.515
	O	5.400	5.601	5.579	5.533	5.528	5.522	5.541	5.532	5.525
	F	5.698	5.579	5.578	5.522	5.508	5.549	5.519	5.517	5.514
	OH	5.507	5.547	5.545	5.523	5.504	5.498	5.525	5.518	5.514
	OF	5.328	5.600	5.596	5.529	5.512	5.502	5.519	5.517	5.519
2	Pristine	6.116	5.591	5.599	5.543	5.535	5.521	5.553	5.599	5.600
	H	5.541	5.513	5.509	5.520	5.499	5.511	5.518	5.526	5.516
	O	5.511	5.572	5.562	5.526	5.525	5.517	5.529	5.518	5.526
	F	5.630	5.549	5.551	5.521	5.502	5.514	5.519	5.525	5.513
	OH	5.520	5.533	5.536	5.524	5.504	5.514	5.521	5.515	5.526
	OF	5.441	5.554	5.561	5.524	5.508	5.517	5.519	5.512	5.530
3	Pristine	6.123	5.583	5.576	5.534	5.532	5.521	5.541	5.598	5.601
	H	5.526	5.516	5.509	5.519	5.504	5.509	5.519	5.521	5.530
	O	5.512	5.575	5.568	5.523	5.511	5.528	5.526	5.525	5.520
	F	5.621	5.549	5.544	5.520	5.506	5.511	5.519	5.524	5.514
	OH	5.503	5.530	5.533	5.520	5.506	5.510	5.521	5.525	5.523
	OF	5.543	5.550	5.551	5.521	5.515	5.508	5.520	5.526	5.525
4	Pristine	6.125	5.578	5.559	5.531	5.525	5.532	5.519	5.542	5.552
	H	5.536	5.517	5.500	5.519	5.509	5.506	5.518	5.528	5.532
	O	5.507	5.578	5.565	5.523	5.528	5.530	5.524	5.525	5.526
	F	5.621	5.550	5.541	5.519	5.507	5.511	------	------	-----
	OH	5.511	5.537	5.523	5.520	5.503	5.513	5.521	5.527	5.520
	OF	5.444	5.554	5.541	5.520	5.510	5.515	------	------	------

Table S3. The energy differences of FM and AFM1, AFM2, and AFM3 with respect to NM phase for Z-C_2NNR, taking the energy of NM phase as zero

Magnetic phase	Magnetic ordering		Energy (meV)
	Edge 1	Edge 2	
NM			0
FM	↑ ↑	↑ ↑	-523.77
AFM1	↑ ↑	↓ ↓	-497.5
AFM2	↑ ↓	↑ ↓	-517.34
AFM3	↑ ↓	↓ ↑	-498.91

Table S4. The calculated binding energy E_b(eV) of C_2NNRs with H, O and F saturated for a series of ribbon widths

C_2NNR / Width	Z-C_2NNR			A1-C_2NNR			A2-C_2NNR		
	H	O	F	H	O	F	H	O	F
1	4.142	7.402	5.146	5.371	7.431	5.332	5.065	6.952	4.321
2	4.154	7.421	5.161	5.376	7.435	5.336	5.068	6.954	4.348
3	4.158	7.421	5.162	5.376	7.435	5.337	5.071	6.957	4.351
4	4.158	7.422	5.162	5.378	7.438	5.337	4.796	6.681	1.962

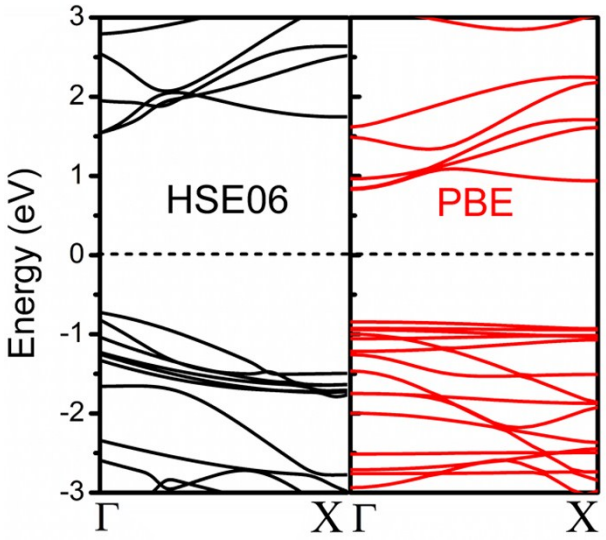

Figure S1. The band structure of H saturated A1-C_2NNR calculated by HSE06 and PBE method respectively.

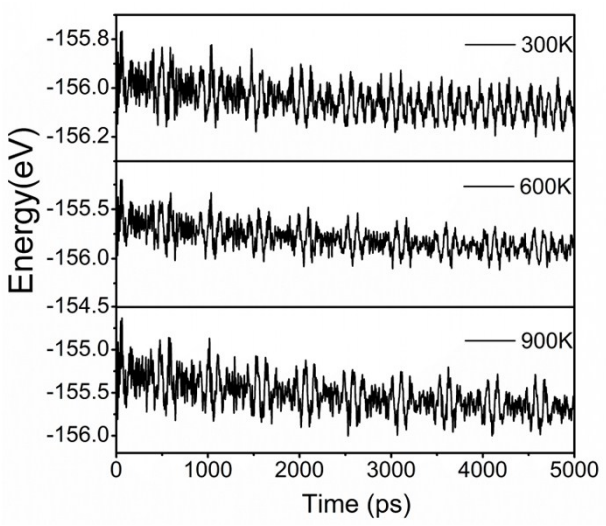

Figure S2. Relationships of total energy and time during 300K, 600K and 900K MD simulations of monolayer C_2N.

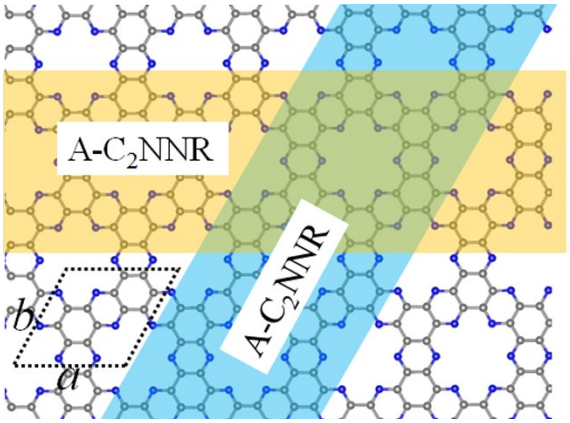

Figure S3. The atomic structure of armchair nanoribbons slicing along a and b direction of unit cell.

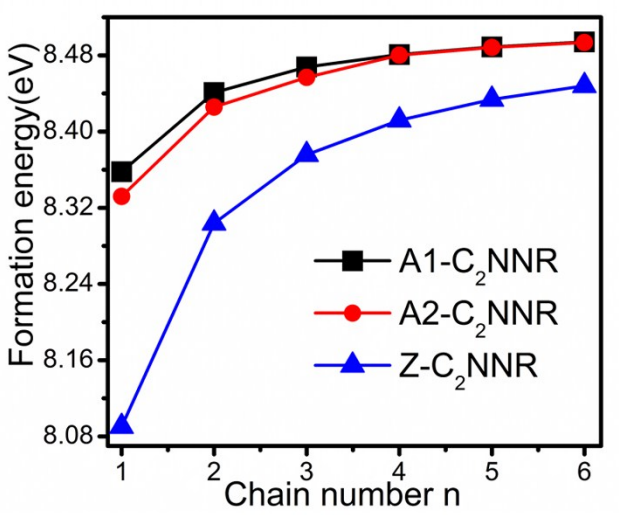

Figure S4. The formation energy of different C_2NNRs depending on the chain number n.

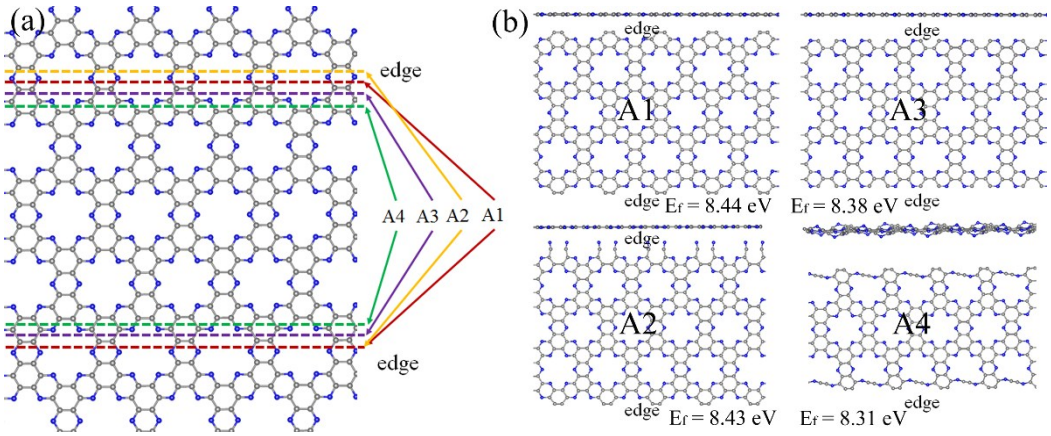

Figure S5. (a) The atomic structure of different armchair nanoribbons, named as A1, A2, A3 and A4 C_2NNRs. (b) The optimized atomic structures of armchair nanoribbons.

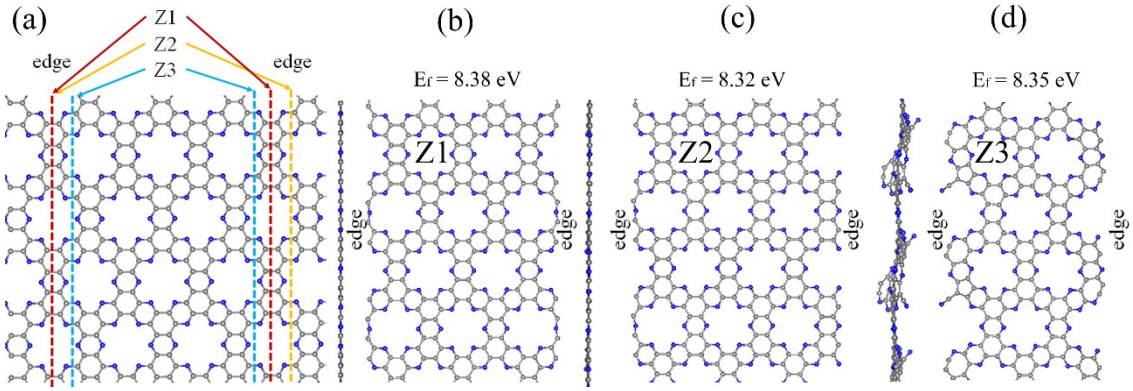

Figure S6. (a) The atomic structure of different zigzag nanoribbons, named as Z-C_2NNRs. The optimized atomic structures of (b) Z1-C_2NNR, (c) Z2-C_2NNR and (d) Z3-C_2NNR.

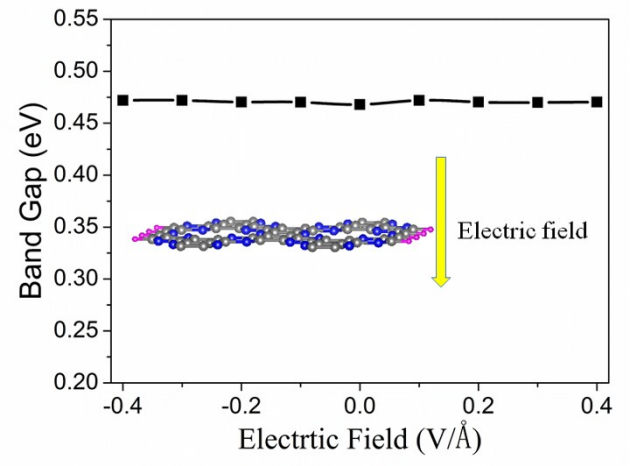

Figure S7. The band gap of H-Z-C_2NNR depending on the vertical electric field.