Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary Materials for:

Tuning the Electronic and Quantum Transport Properties of Nitrogenated Holey Graphene Nanoribbons

Table S1: Relative Energies of armchar and zigzag ($n_{a/z}$) C_2N-hNRs in different Magnetic states.

$n_{a/z}C_2N$-hNRs	NM(meV)	AFM(meV)	FM(meV)
3A	**22.6**	**19.2**	**0**
7A	**14.1**	**0.02**	**0**
11A	**18.6**	**10.02**	**0**
4Z	**0**	**0.01**	
10Z	**0**	**0.13**	
12Z	**0**	**0.09**	

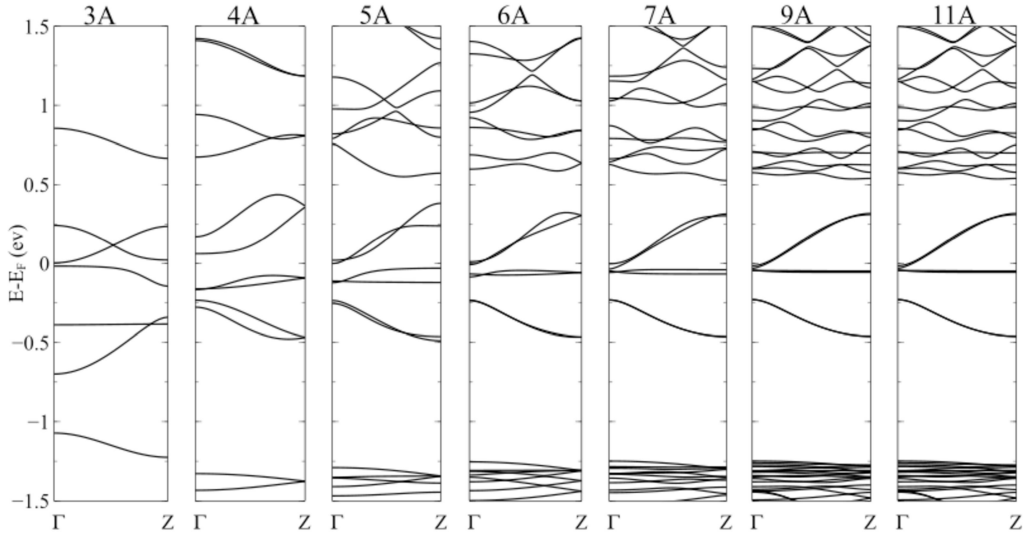

Figure S1: Evolution of band structures for 3A, 4A, 5A, 6A, 7A, 9A and 11A C_2N-*h*NRs, respectively.

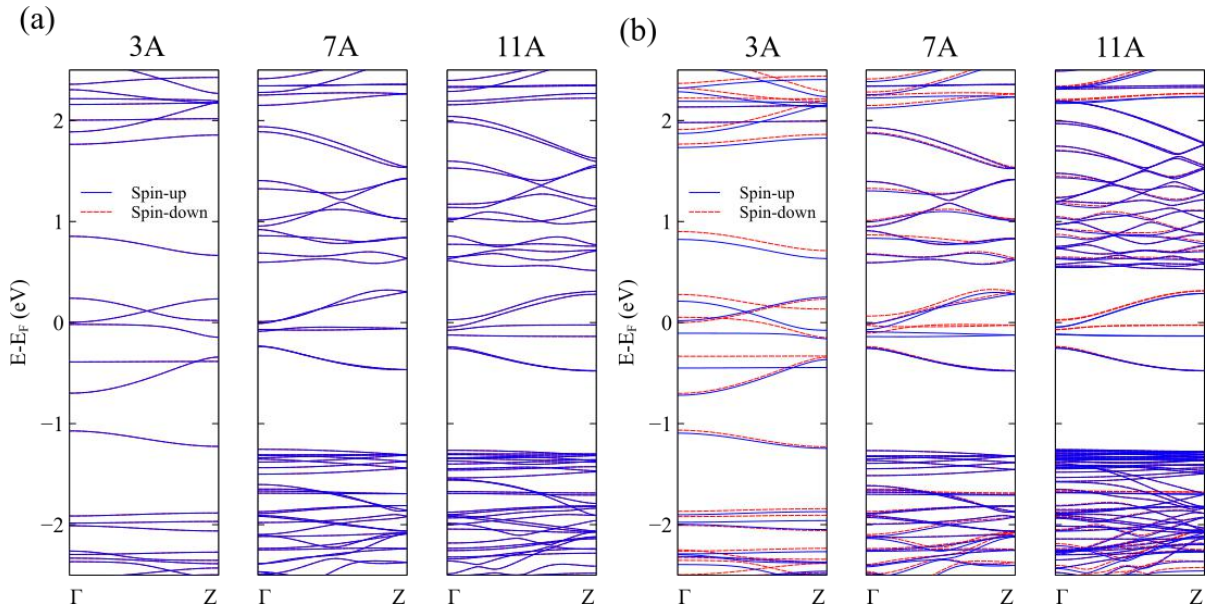

Figure S2: (a) and (b) Evolution of band structures for 3A, 7A, and 11A C_2N-*h*NRs for antiferromagnetic (AFM) and ferromagnetic (FM) states, respectively.

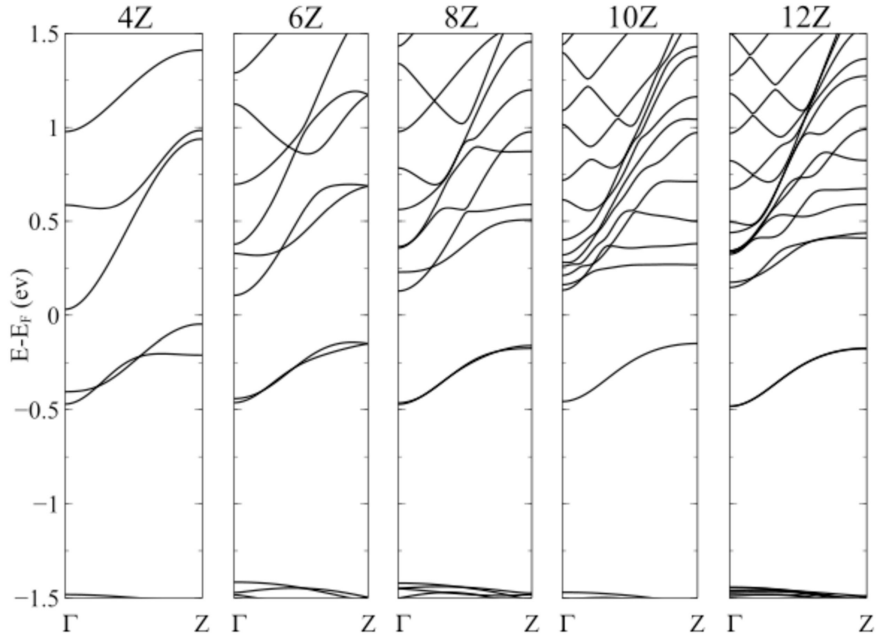

Figure S3: Evolution of band structures for 4Z, 6Z, 8Z, 10Z and 12Z C_2N-*h*NRs, respectively.

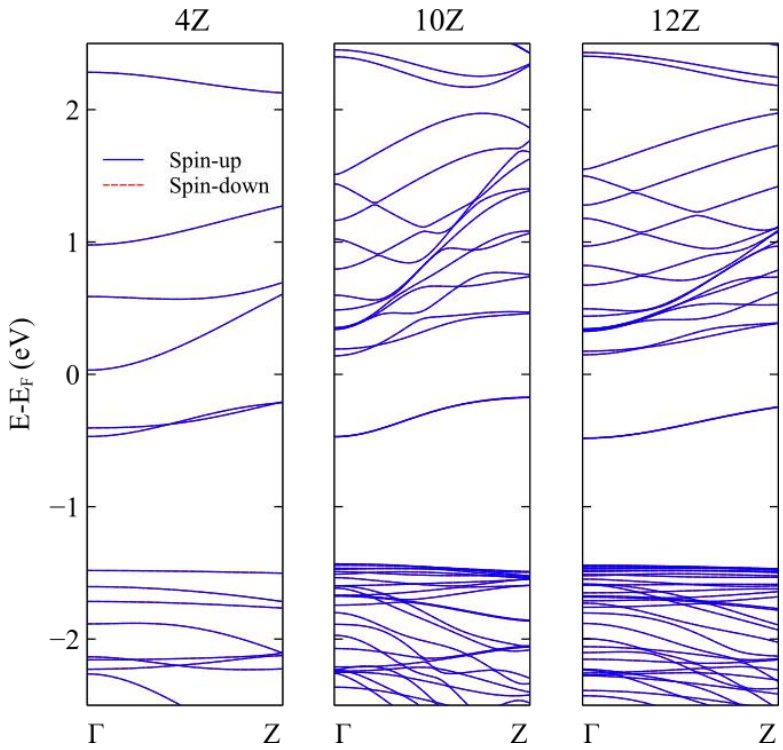

Figure S4: Evolution of band structures of for antiferromagnetic (AFM) for 4Z, 10Z and 12Z C_2N-*h*NRs, respectively.

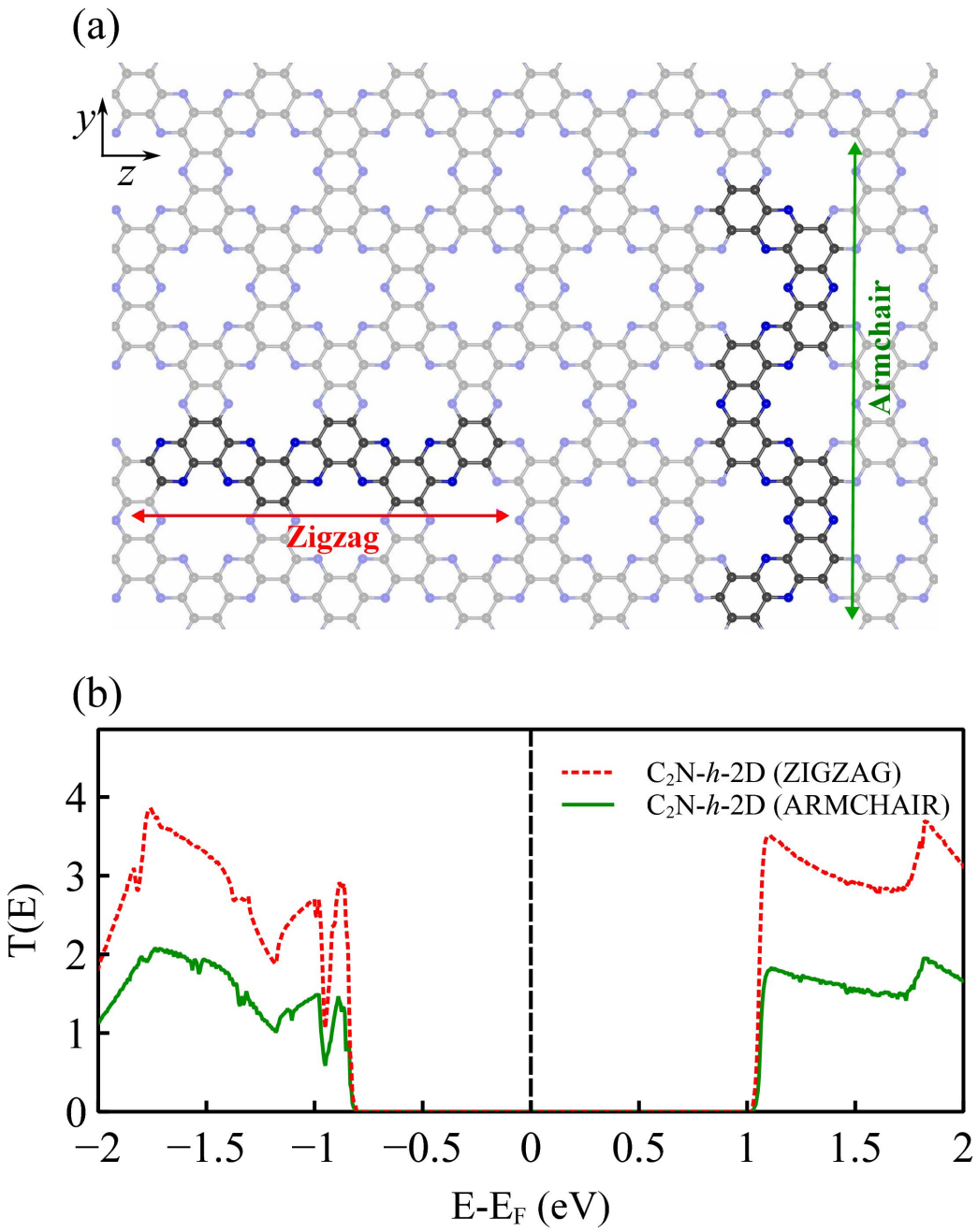

Figure S5: (a) Schematic view of the C_2N*h*-2D with labelled armchair and zigzag directions. (b) Transmission spectra of the C_2N*h*-2D for each direction.

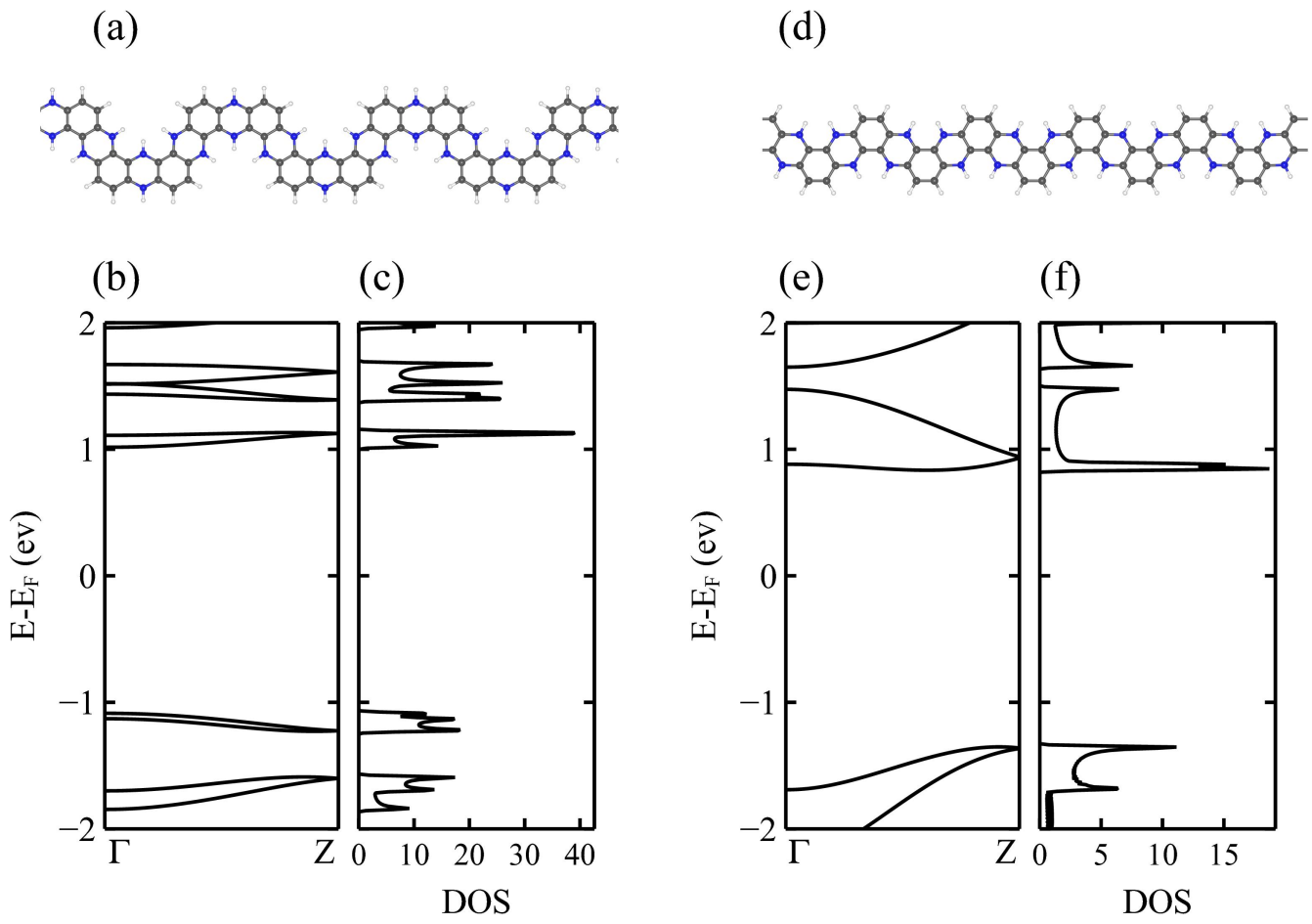

Figure S6: (a) and (d) Schematic view; (b) and (e) calculated band structures and (e) and (f) density of states (DOS) of the narrowest armchair and zigzag C_2N*h*NRs, respectively.

Supplementary Note 1 | Sample Input Files for Calculations.

1) Siesta

Version: 3.2-pl-5

4ZC$_2$N-*h*-NR SCF input file:

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SystemName          4-z
SystemLabel         4-z.file

LatticeConstant             1.00 Ang

%block LatticeVectors
      15.936505    0.000000    0.000000
       0.000000   30.246551    0.000000
       0.000000    0.000000    8.438071
%endblock LatticeVectors

NumberOfSpecies         3
NumberOfAtoms           42

%block ChemicalSpeciesLabel
  1   1  pseudos/H-gga
```

```
  2    6  pseudos/C-gga

  3    7  pseudos/N-gga

%endblock ChemicalSpeciesLabel



AtomicCoordinatesFormat Ang



%block AtomicCoordinatesAndAtomicSpecies

        7.96839552   12.75967562    2.81335136     3

        7.96859021   19.96203911    7.01018536     3

        7.96836749   15.14275158    7.01644177     3

        7.96834734   10.31878083    7.01096619     3

        7.96864459   17.52559324    2.81209156     3

        7.96844720   10.31874820    1.42924311     3

        7.96854933   17.52579770    5.62782336     3

        7.96846649   15.14239122    1.42361585     3

        7.96836170   12.75989564    5.62665312     3

        7.96873344   19.96176024    1.42959976     3

        7.96835353   11.50678911    0.70108191     2

        7.96852979   18.72031714    4.94148415     2

        7.96839667   13.99429580    0.72034051     2
```

7.96845815	21.20501773	4.92386683	2
7.96833166	12.72367933	6.95999126	2
7.96856317	19.98862209	2.81962186	2
7.96834775	11.56293324	3.49829328	2
7.96846441	18.77608769	7.73914167	2
7.96829165	9.07597555	3.51586407	2
7.96844438	16.29088285	7.71990020	2
7.96830499	10.29276235	5.62014989	2
7.96854941	17.56062095	1.47937889	2
7.96834686	10.29262409	2.82007945	2
7.96847883	17.56086567	6.96056762	2
7.96833085	11.56298065	4.94191419	2
7.96850804	18.77572951	0.70070404	2
7.96826684	9.07600532	4.92432853	2
7.96849397	16.29052370	0.72014653	2
7.96836877	12.72325804	1.48009917	2
7.96850643	19.98881556	5.62014046	2
7.96832115	11.50708194	7.73894329	2
7.96856958	18.72020815	3.49830303	2
7.96835644	13.99469588	7.71963746	2

```
      7.96848031   21.20491566    3.51570557     2

      7.96844140   20.86483613    7.48192541     1

      7.96826449    9.41522810    7.48251080     1

      7.96832085    9.41522218    0.95745964     1

      7.96848847   20.86451693    0.95788196     1

      7.96845328   22.16241230    5.47571767     1

      7.96827252    8.12027286    2.96081626     1

      7.96824558    8.12013047    5.47921334     1

      7.96847515   22.16210951    2.96350090     1

%endblock AtomicCoordinatesAndAtomicSpecies
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2) Nanodcal

Electrode SCF input file:

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system.name = ' 4zig_elec '

system.spinType = ' NoSpin '

system.orbitalType = ' DZP '

system.atomCoordinateFormat = ' cartesian '

system.atomFile = ' ./4zigelec.xyz '
```

```
system.centralCellVectors =' [15.996000, 17.642600,    8.536120] '



calculation.name = ' scf '
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Central region SCF input file:

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system.name =  ' 4zig_scat '

system.spinType = ' NoSpin'

system.orbitalType = ' DZP '



system.centralCellVectors = [15.996000 , 17.642600, 51.216720]

system.atomFile = ' scat.xyz '



calculation.name = ' scf '
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