

**Supporting Information For the Article in Physical Chemistry Chemical Physics:
Electronic Structures and Transport Properties in Fluorinated Boron Nitride
Nanoribbons**

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1. Atomic structures for 8-ZBNNR- i F ($i=2-8$)

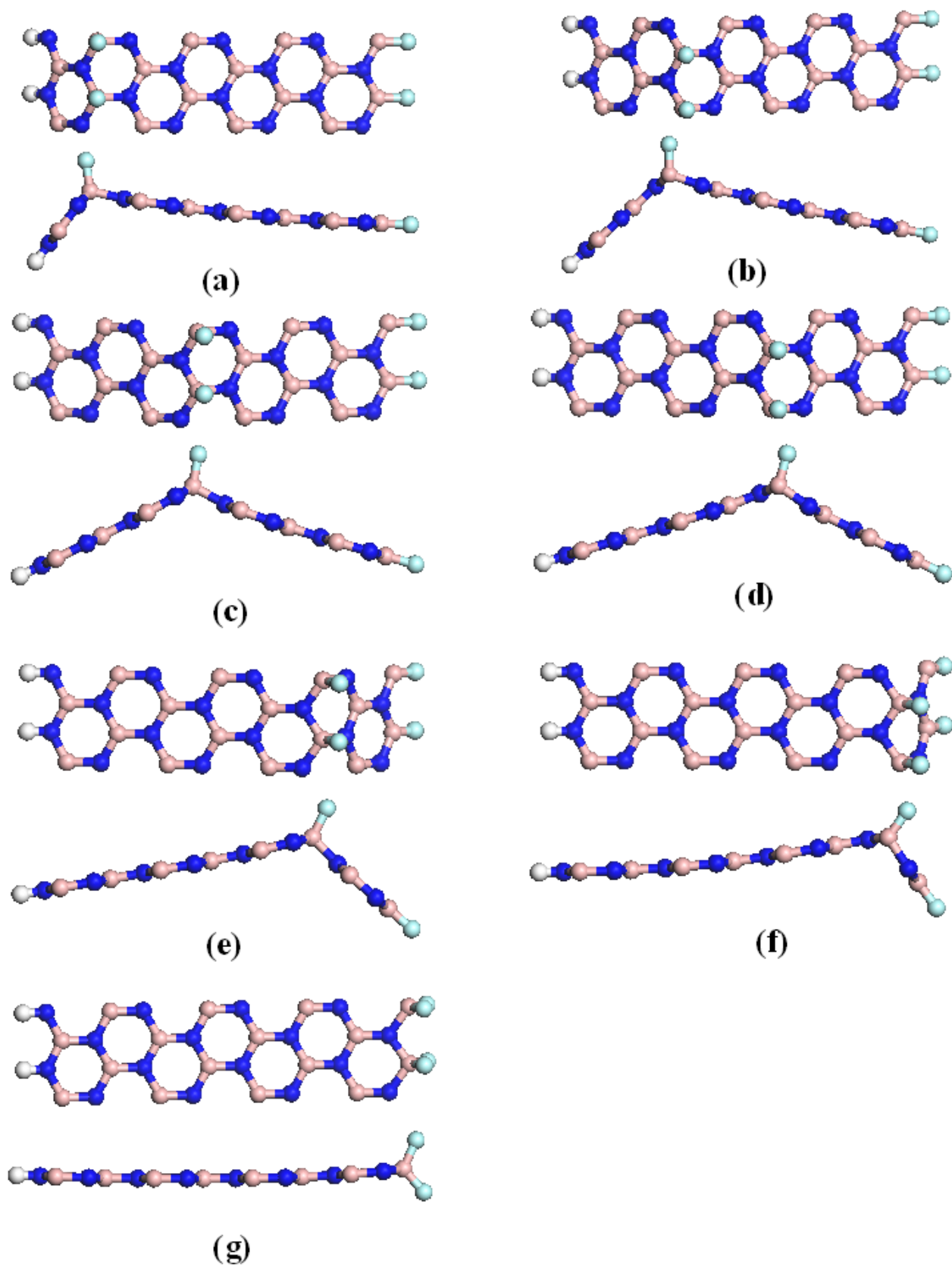


Figure S1. (Color online) (a)-(g) : The top and side views of the 8-ZBNNR- i F ($i=2-8$).

2. Band structures for 8-ZBNNR- i F ($i=3-6$)

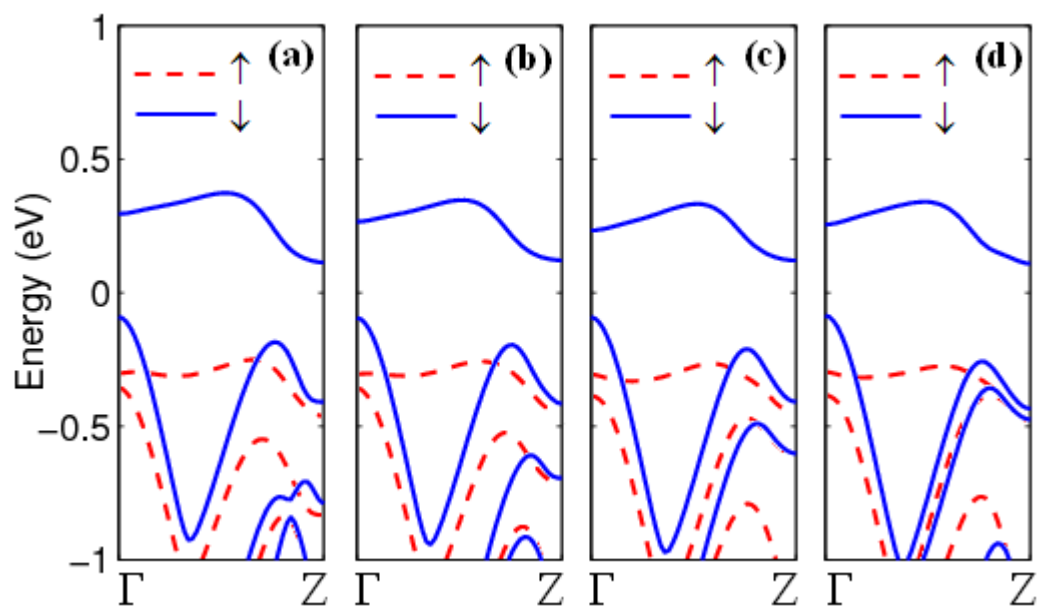


Figure S2. (Color online) The calculated band structures: (a)-(d) correspond to 8-ZBNNR-3F, 8-ZBNNR-4F, 8-ZBNNR-5F, and 8-ZBNNR-6F, respectively.

3. Electronic properties and I-V curves for 8-ZBNNR-3F (ground state)

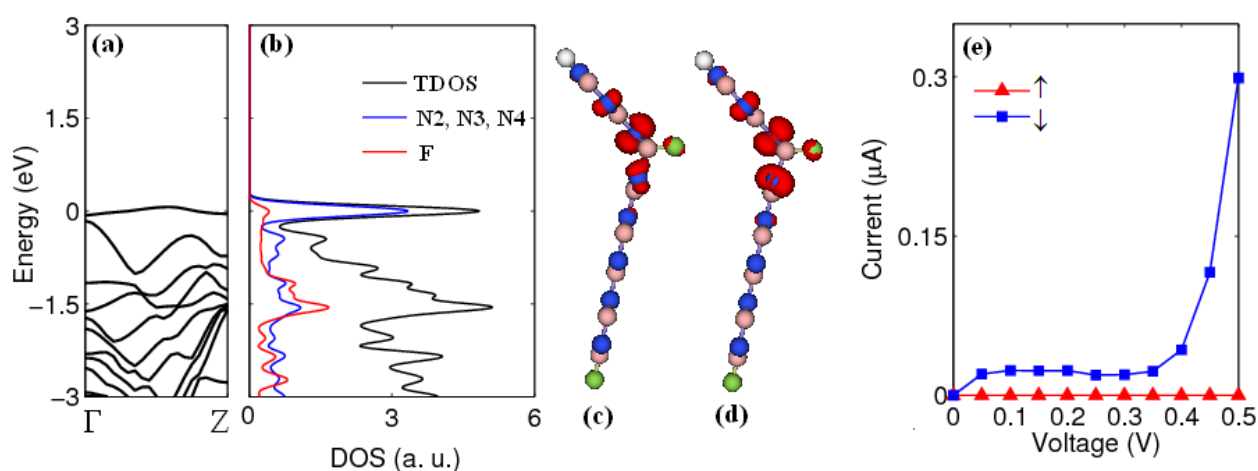


Figure S3. (Color online) (a) and (b) correspond to spin-unresolved band structure and DOS of 8-ZBNNR-3F, respectively. (c) : The wave function of partial-filled band (Γ point). (d): The difference between the spin up and down electron density (The iso-value is 0.005 1/\AA^3). (e): Calculated current as a function of the applied bias for 8-ZBNNR-3F.

From the Fig. S3(a), we can find that there is a partial-filled band near the Fermi level for 8-ZBNNR-3F, which is mainly contributed by three N atoms (N2, N3, and N4). This is clearly illustrated by the Γ point wave function of partial-filled band [see Fig. S3(c)]. The difference between spin-up and spin-down electron density indicates that the un-paired spin is strongly localized on the N atoms surrounding the adsorption site [see Fig. S3(d)]. Mulliken population analysis shows that the 8-ZBNNR-3F has a total magnetic moment of $m \approx 1\mu_B$ per unit cell. More specially, the contributions of these nitrogen atoms N2, N3, and N4 to the magnetic moment are $0.13 \mu_B$, $0.44 \mu_B$, and $0.31 \mu_B$, respectively. The I-V current for 8-ZBNNR-3F is shown in Fig. S3(e). From the picture, we can find that the spin-down current almost keep unchanged due to the presence of spin-down band gap. When the bias is larger than 0.35 V, the current increases quickly.

8-ZBNNR- i F ($i = 2, 4-7$) and its corresponding electron states are localized, which drives spontaneous spin polarization. The un-paired spin is strongly localized on the N atoms surrounding the adsorption site. For 8-ZBNNR-2F, the contributions of nitrogen atoms N1, N2, and N3 to the magnetic moment are $0.14 \mu_B$, $0.48 \mu_B$, and $0.31 \mu_B$, respectively; For 8-ZBNNR-4F, the contributions of nitrogen atoms N3, N4, and N5 to the magnetic moment are $0.12 \mu_B$, $0.43 \mu_B$, and $0.31 \mu_B$, respectively; For 8-ZBNNR-5F, the contributions of nitrogen atoms N4, N5, and N6 to the magnetic moment are $0.12 \mu_B$, $0.43 \mu_B$, and $0.31 \mu_B$, respectively; For 8-ZBNNR-6F, the contributions of nitrogen atoms N5, N6, and N7 to the magnetic moment are $0.12 \mu_B$, $0.44 \mu_B$, and $0.31 \mu_B$, respectively; For 8-ZBNNR-7F, the contributions of nitrogen atoms N6, N7, and N8 to the magnetic moment are $0.12 \mu_B$, $0.47 \mu_B$, and $0.31 \mu_B$, respectively; For 8-ZBNNR-8F, the un-paired spin mainly concentrates on N7, N8, and two F atoms attached on the edge B atom, and their corresponding magnetic moments are $0.14 \mu_B$, $0.58 \mu_B$, and $0.25 \mu_B$, respectively.