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Supplementary Information

Possibility of Spin-polarized Transport in Edge Fluorinated Armchair Boron Nitride Nanoribbons

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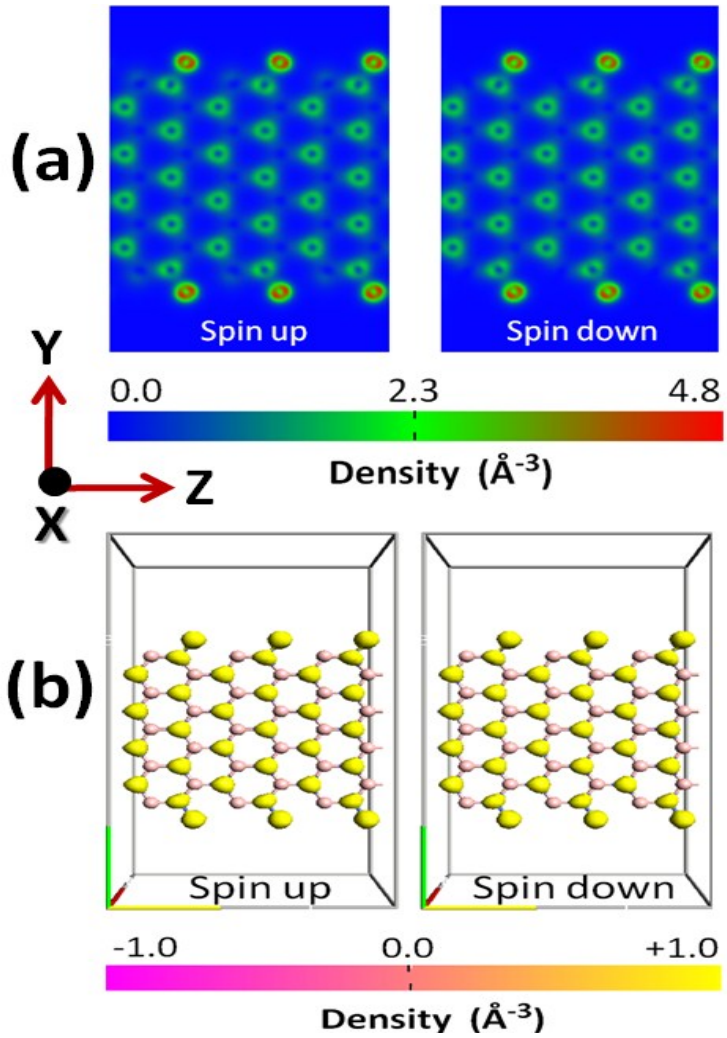

Fig. S1: (Color online). The real space distribution of calculated electron densities corresponding to spin up and spin down electrons for 9-ABNNR$_{FN}$ is presented in the form of (a) Contour and

(b) Isosurface. The corresponding density scale is shown by a tricolored rectangular horizontal strip situated at the bottom. In figure (b), the electron density is plotted corresponding to isovalue 1 (au). In order to display the distinct change (if any) between spin up and spin down electron densities at ribbon edges, ribbon configurations are not shown in figure (a). B, N and F atoms are same in shape, size and color as that of represented in figure1. The ABNNRs are modeled with periodic boundary conditions along *z*- axis whereas x and y directions are confined.

We found that the fluorination of the zigzag ribbons is energetically more favorable than that of the ABNNRs. The calculated values for the ribbons with fluorinated zigzag edges are given below for comparison with edge-fluorinated ABNNRs (tabulated in main text).

Table S1: Calculated **cohesive energy Ec** (eV) as a function of ribbon width for fluorinated ZBNNR structures.

Ribbon width N_Z	E_c(eV)		
	$ZBNNR_{FB}$	$ZBNNR_{FBN}$	$ZBNNR_{FN}$
6	-9.588	-9.305	-9.283
8	-9.734	-9.506	-9.501
10	-9.825	-9.634	-9.636

Table S2: Calculated **binding energy E_B** (eV) per F-atomas a function of ribbon width for fluorinated ZBNNR structures.

Ribbon width N_Z	E_B(eV)		
	$ZBNNR_{FB}$	$ZBNNR_{FBN}$	$ZBNNR_{FN}$
6	-9.450	-7.535	-5.483
8	-9.479	-7.551	-5.511
10	-9495	-7.558	-5.527