Supporting Information

Robust Half-Metallic Ferromagnetism and Curvature Dependent Magnetic Coupling in Fluorinated Boron Nitride Nanotubes

Chunsheng Guo[a],* Yu Zhou[a], Xin-Qiang Shi[b], Li-Yong Gan[a],* Hong Jiang[c],* and Yong Zhao[a,d]

[a]*Key Laboratory of Advanced Technology of Materials (Ministry of Education), Superconductivity and New Energy R&D Center, Mail Stop 165#, Southwest Jiaotong University, Chengdu, Sichuan 610031, China*

[b]*Department of Physics, South University of Science and Technology of China, Shenzhen 518055, China.*

[c] *Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Rare Earth Materials Chemistry and Application, College of Chemistry and Molecular Engineering, Peking University, 100871 Beijing, China*

[d]*School of Materials Science and Engineering, University of New South Wales, Sydney, 2052 NSW, Australia*

1. Little dependence of the net moment induced by fluorine adsorption on the axial strain

The net moment induced by fluorine adsorption calculated by HSE06 functional depends little on the small axial strain. As denoted in Figure S1, the equivalent HSE06 lattice constant of the (8,0) F-BN nanotube is 0.02 Å larger than the LDA one, while the net moment is always 1 μ_B. Even with up to 3% compressive or tensile strain, the magnetic moment per unit cell is always maintained in our simulations.

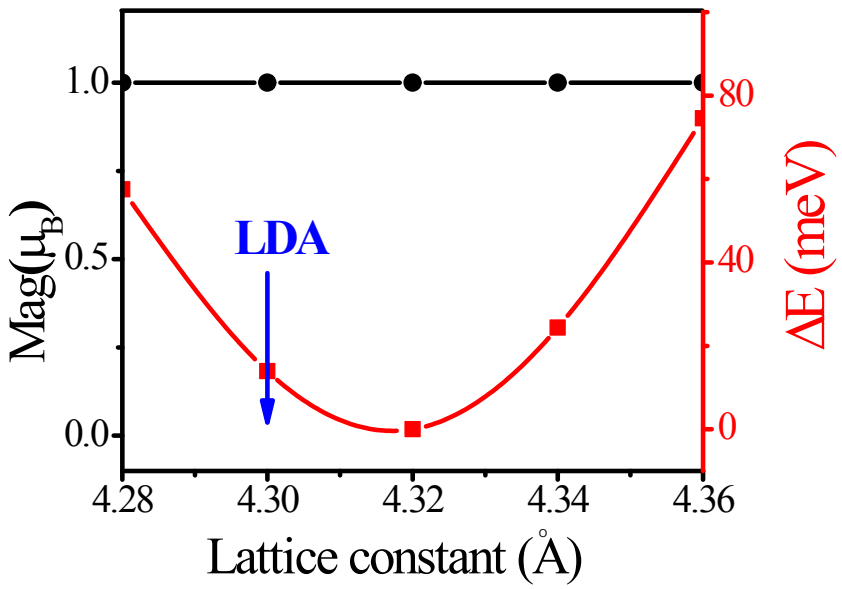

Figure S1. Magnetic moment (black) and relative total energy (red) vs. lattice constant, respectively, for (8,0) F-BN nanotube calculated with HSE06. The total energy of the nanotube with equivalent lattice constant is set to zero. The LDA equivalent lattice constant is 4.30, marked with a blue arrow.

2. Spin density plot of nanoribbon and sheet

The spin density of nanoribbon is exactly the same to the distribution of the nantoubes, a little more on N1 along the long axis and less on N2 and N3, and due to the symmetry the spin density is equally distributed on the three N atoms, as shown in Figure S2. The spin density is highly localized on the three N atoms near the adsorption site.

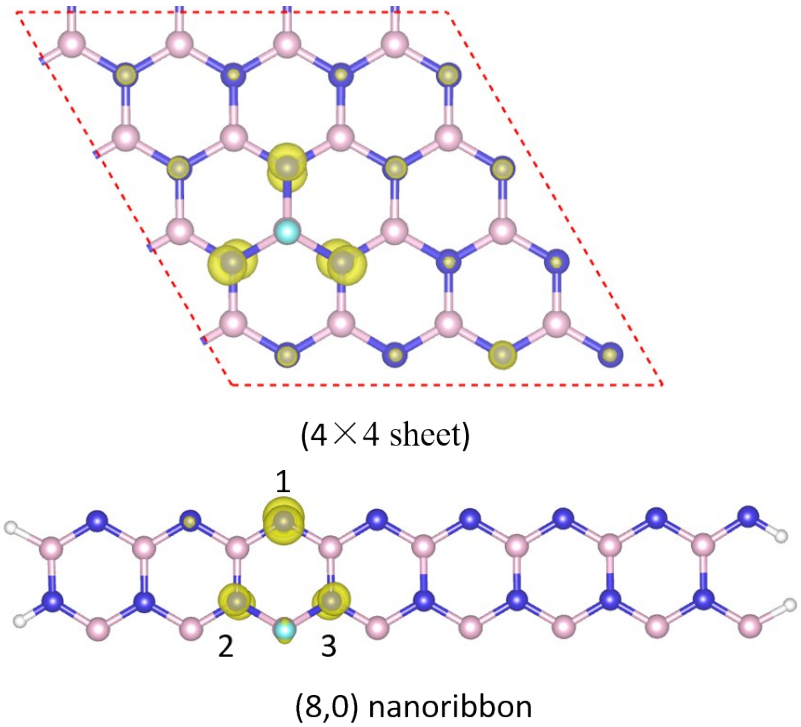

Figure S2. Spin density plots (0.01e/Å^3 iso-surface plot) of (4×4) sheet and (8,0) nanoribbon.