Electronic Supplementary Information

Electrical Properties of O-Self-Doped Boron-Nitride Nanotubes and the Piezoelectric Effects of their Freestanding Network Film

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Theoretical simulation

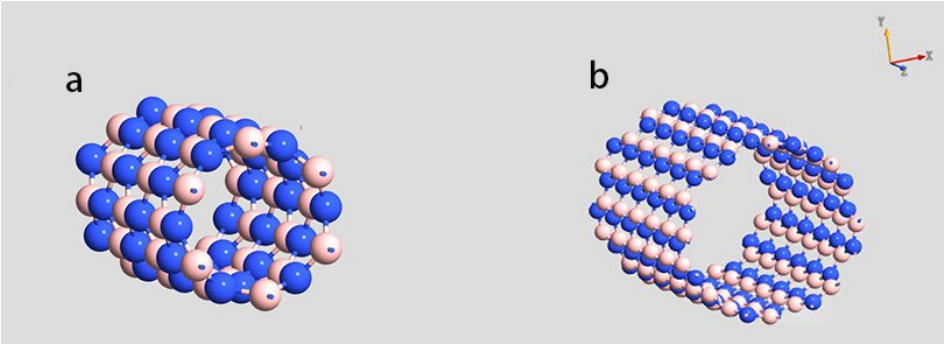

Figure S1 Ball-stick models of (a) (6,0) BNNT and (b) (8,8) BNNT; all the models were built using Virtual Nanolab (free academic version).

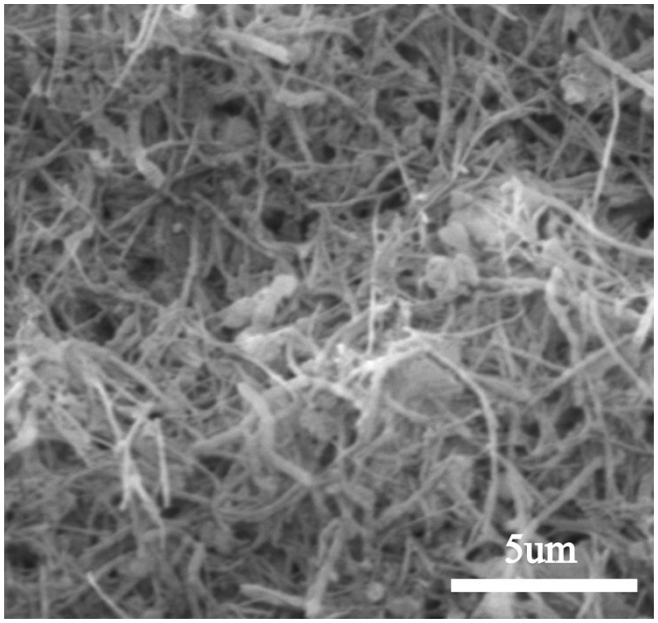

Figure S2 SEM images of O-self-doped BNNTs network film

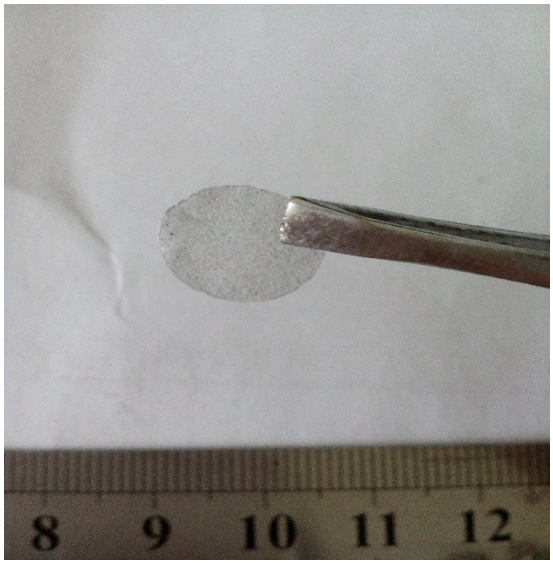

Figure S3 the physical map of the BNNTs freestanding network film

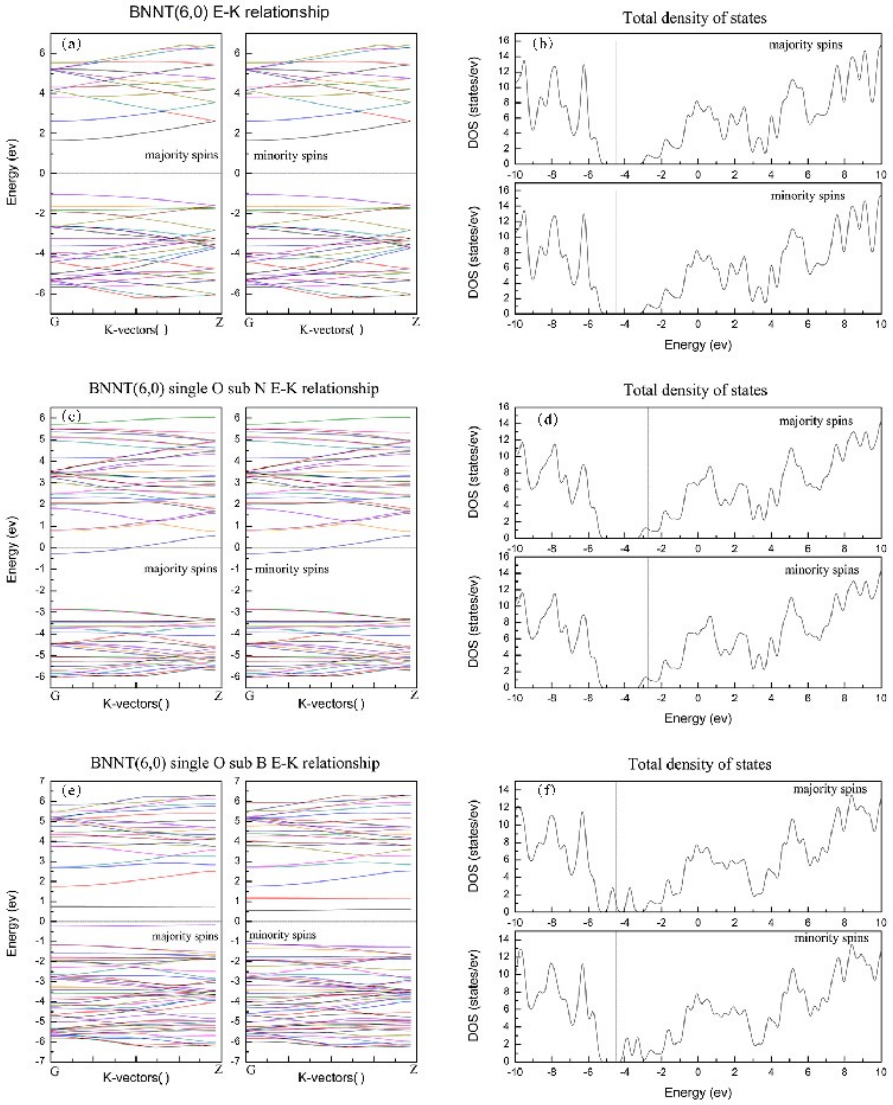

Figure S4 (a), (b) DOS and the band gaps of the pure, (c) (d) O_N-doped, and (e) (f)

O_B-doped (6,0) BNNTs.

Two impurity energy levels are located in the band gap of the O_B-doped (6,0) zigzag BNNTs with different spintronic properties (Figure S1 (e) and (f)). For the majority spins, the Femi energy level is located across two impurity energy levels, while the minority spins have different states that are located at the bottom of the conduction band. Both spins lead to a decrease in the band gap of the NT, and the NT system has spin polarization and increased conductivity compared with that of the pure NT. The oxygen substituted for boron in the lattice has two extra electrons because oxygen possesses two more valence electrons than boron. The periodic arrangement in the crystals leads to a periodic arrangement of the electron wave functions, enhancing the impurity in the lattice, which leads to the impurity energy levels. When nitride is substituted by an oxygen atom, one extra, free electron is present, and only one impurity energy level is formed near the valance band (Figure S1 (c) and (d)). In addition, O substituting for N leads to a decrease in the band gap because the Femi energy level lies at the bottom of the valence band, which can be regard as a metallic band gap (Figure S1). The majority spins in the DOS of the O_N-doped BNNT and the minority spins in the DOS of the O_B-doped BNNT are asymmetric, leading to spin polarization and ferromagnetism in the BNNTs.

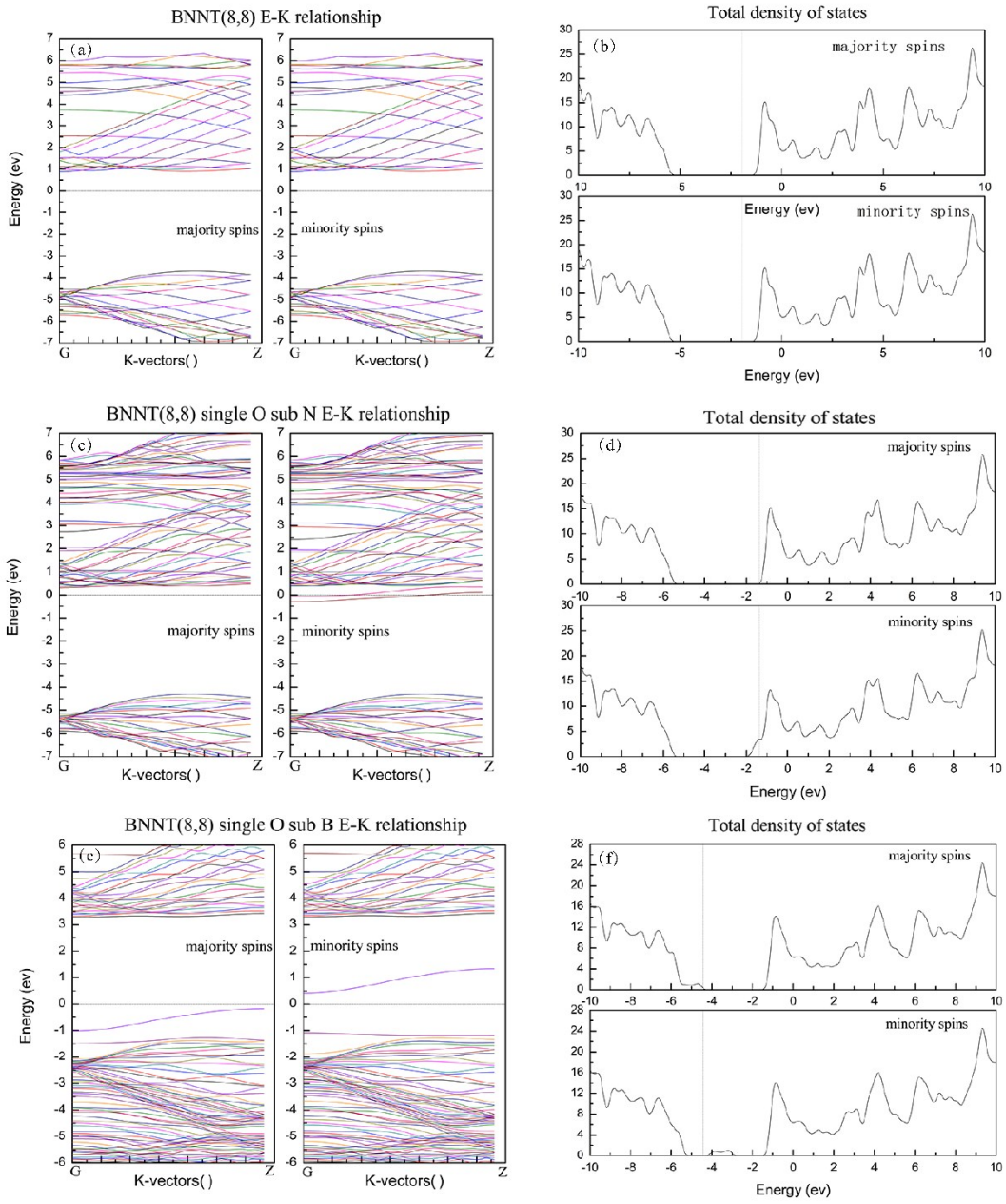

Figure S5 DOS and the band gaps of the pure, O_N-doped and O_B-doped (8,8) armchair BNNTs.

For the armchair (8,8) BNNT, the band gap and DOS of the pure (8,8) BNNT is the same as the (6,0) BNNT (Figure S1(a)(b) and Figure S2 (a) (b)), respectively. The band gap of both the O_B-doped (8,8) BNNT and the O_N-doped (8,8) BNNT decreases in comparison with that of the pure BNNT. However, the energy level and DOS are quite different owing to the different electron spins. The Femi energy level lies at the

valence band for the minority spins in the O_N-doped (8,8) BNNT; however, the Femi energy level is slightly above the valance band for the majority spins in the O_B-doped (8,8) (Figure S2 (c) and (d)). Two impurity energy levels lie within the band gap of the minority spins in the O_B-doped (8,8) BNNT, and the Femi energy level is slightly below the conduction band for the majority spins in the O_B-doped (8,8) BNNT (Figure 6 (e) and (f)).