Supporting information to

Band Gap Opening and Semiconductor-metal Phase Transition in (n, n) Single-Walled Carbon Nanotubes with Distinctive Boron-Nitrogen Line Defect

Ming Qiu,[a,b] Yuanyuan Xie, [a] Xianfeng Gao, [a] Jianyang Li, [a] Yelin Deng, [a] Dongsheng Guan, [a] Lulu Ma [a] and Chris Yuan[a,*]

[a]Department of Mechanical Engineering, University of Wisconsin Milwaukee, Wisconsin 53211, USA

[b]School of Physics and Electronic Science, Changsha University of Science and Technology, Changsha 410114, China·

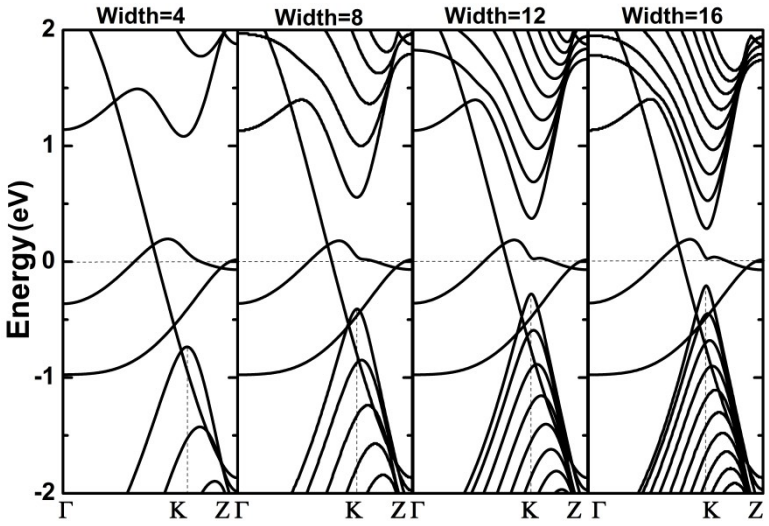

Fig. S1. The band structures of decorated ZGNRs with different widths 4, 8, 12 and 16.

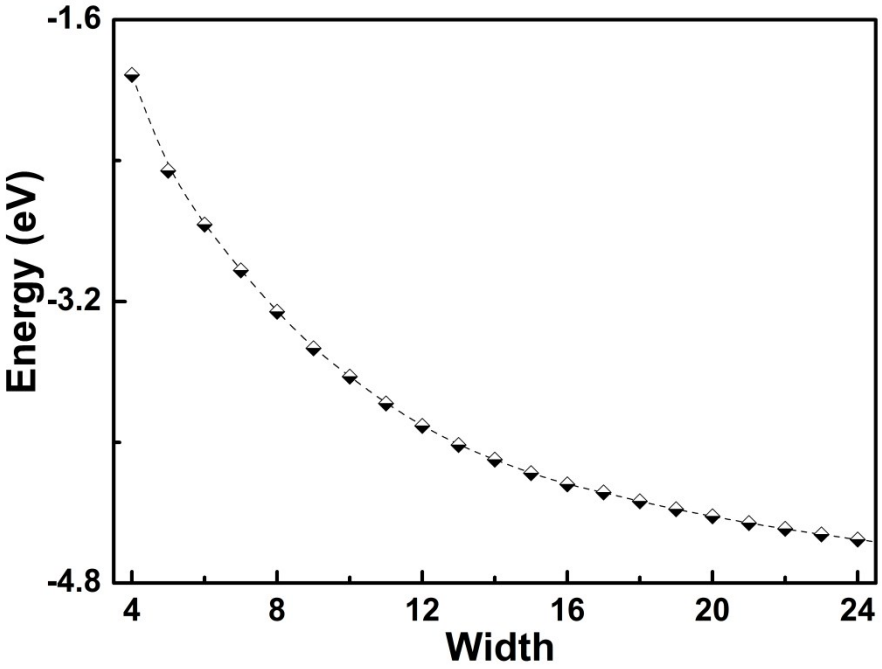

Fig. S2. The evolution of formation energy with different widths from 4 to 24.

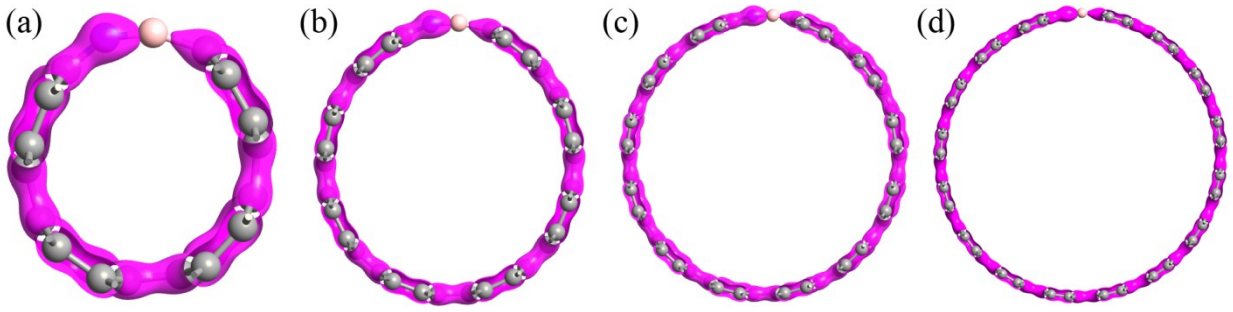

Fig. S3. The electron density of (a) 4bn@CNT, (b) 8bn@CNT, (c) 12bn@CNT and and (d) 16bn@CNT.

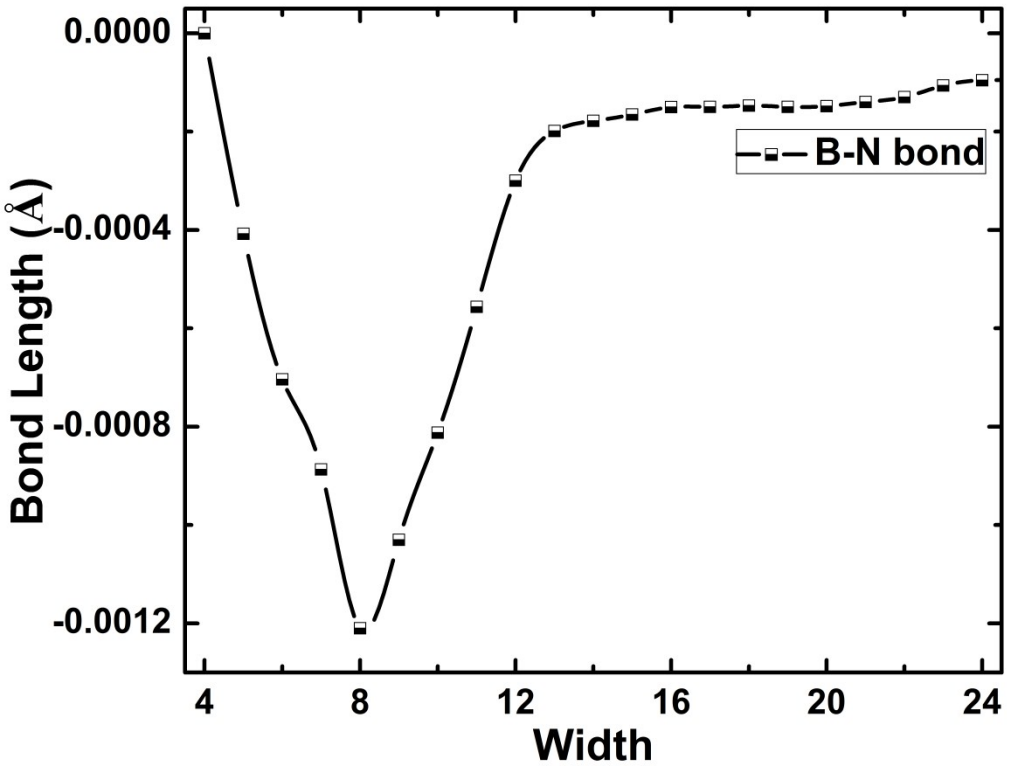

Fig. S4. The increasement of B–N bond on the bn@CNTs with the widths 4 to 24.

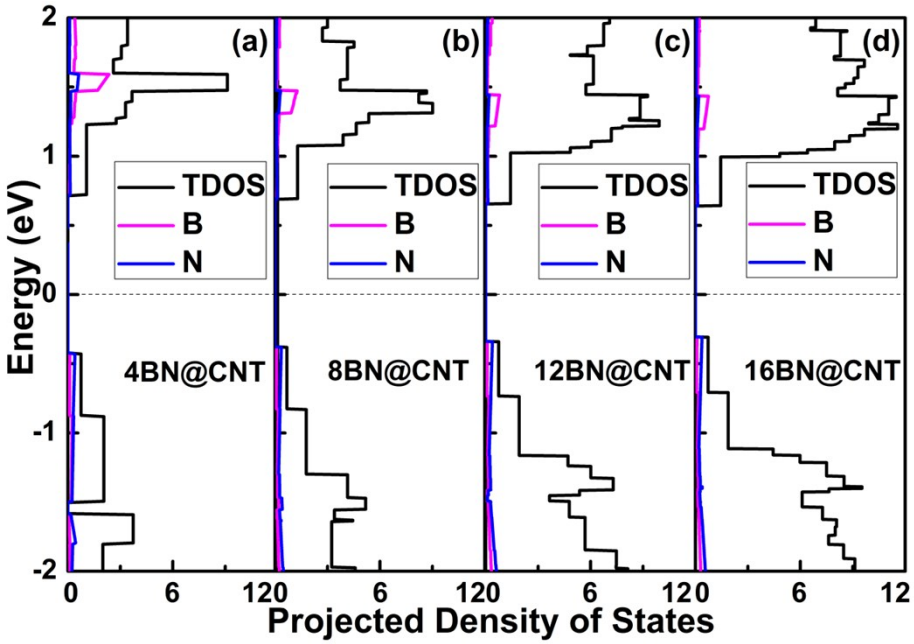

Fig. S5. The projected density of states of (a) 4bn@CNT, (b) 8bn@CNT, (c) 12bn@CNT, and (d) 16bn@CNT. TDOS is the total density of states. B (N) is the Projected density of states on the B (N) atom.

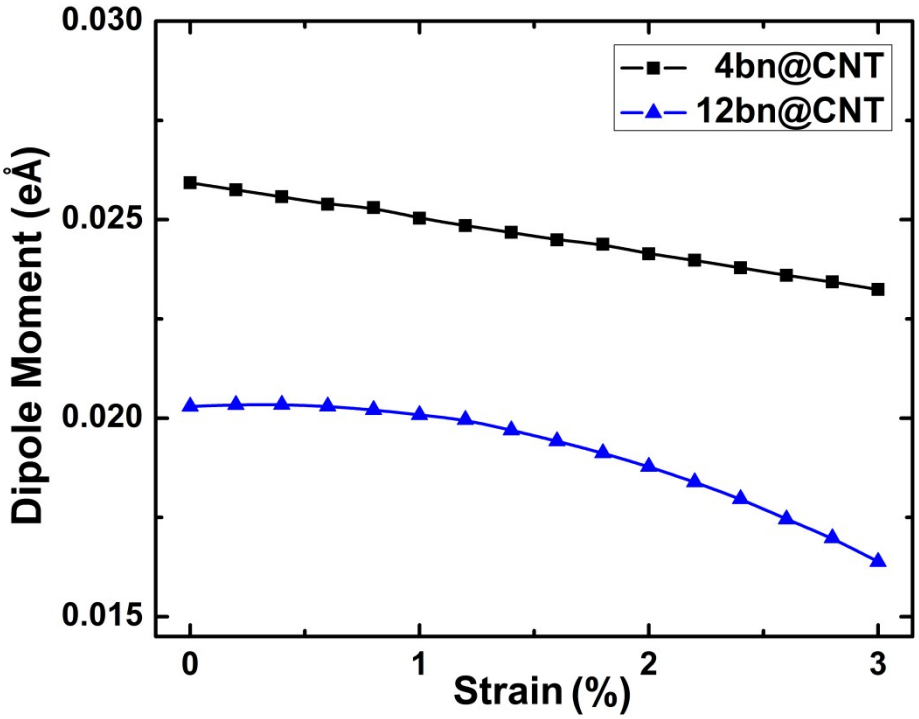

Fig. S6. The evolution of dipole moments of 4bn@CNT and 12bn@CNT along the *y* axis under uniaxial compressive deformation.

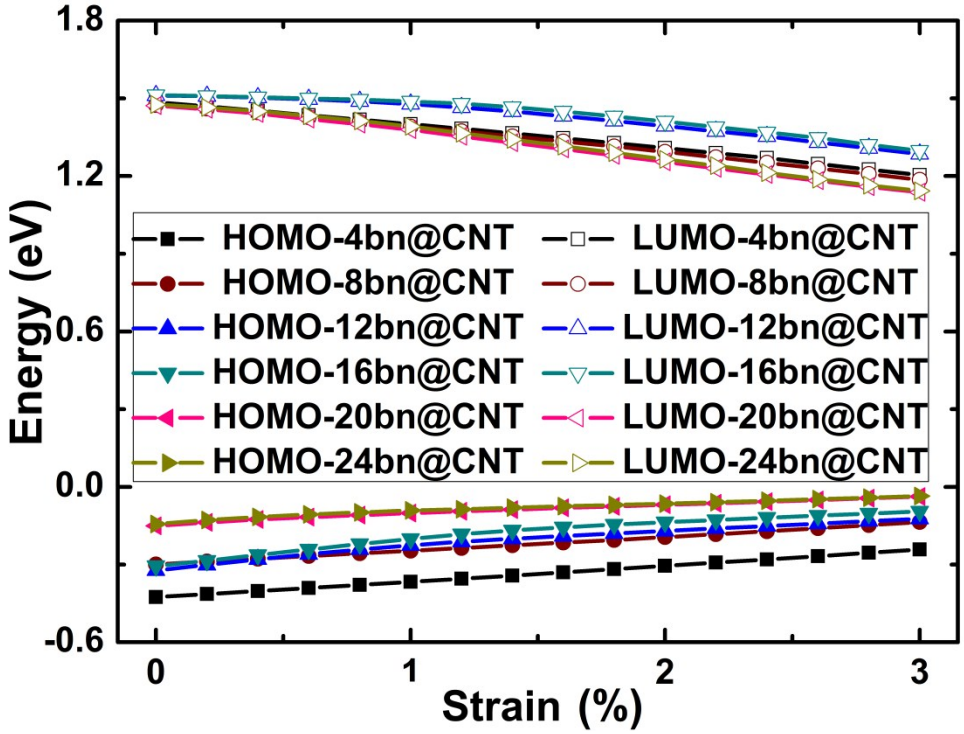

Fig. S7. The evolution of frontier orbitals HOMO and LUMO of different bn@CNTs under uniaxial compressive deformation.

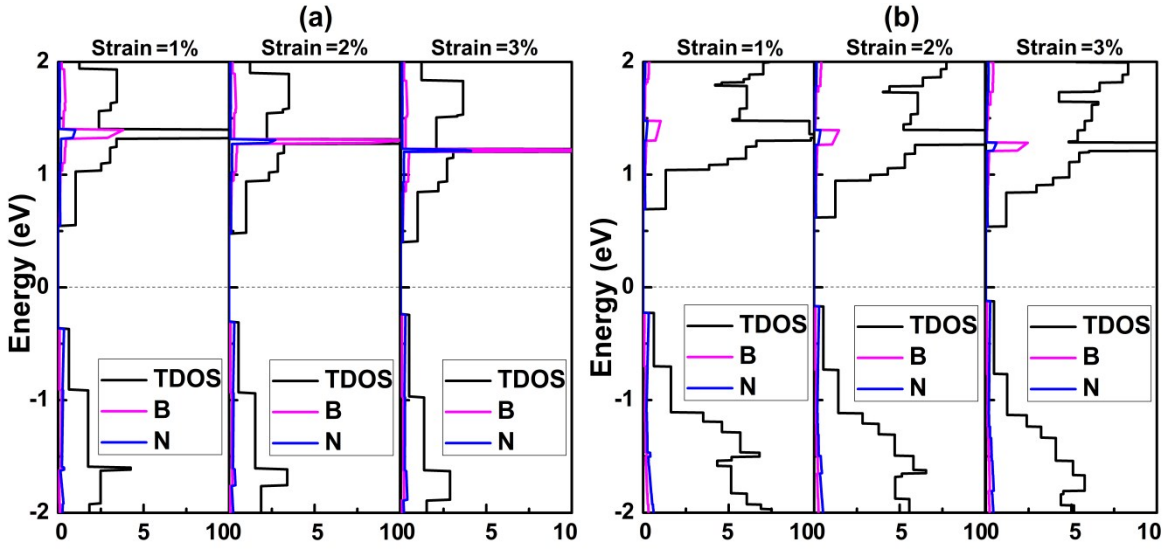

Fig. S8. The projected density of states of (a) 4bn@CNT and (b) 12bn@CNT under uniaxial compressive deformation. TDOS is the total density of states. B (N) is the Projected density of states on the B (N) atom.

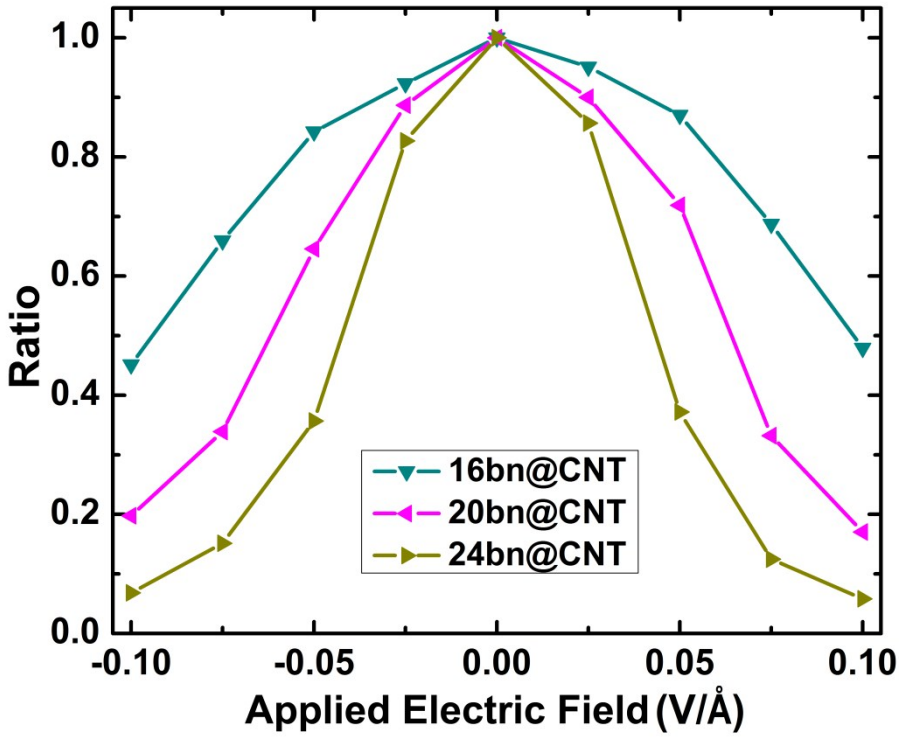

Fig. S9. The ratios, $R = {}^{G_{Electric\ field}}/_{G_0}$, of different bn@CNTs under the electric field applied along the x axis. The $G_{Electric\ field}$ is the band gap under the applied electric field and G_0 is the band gap without applied electric field.

	-0.10 V/Å	-0.01 V/Å	0 V/Å	0.01 V/Å	0.10 V/Å
HOMO					
LUMO					

Fig. S10. The eigenstates HOMO and LUMO of the 16bn@CNT at the applied electric fields of 0, ±0.01 and ±0.10V/Å.