A Fully Tunable Single-Walled Carbon Nanotube Diode

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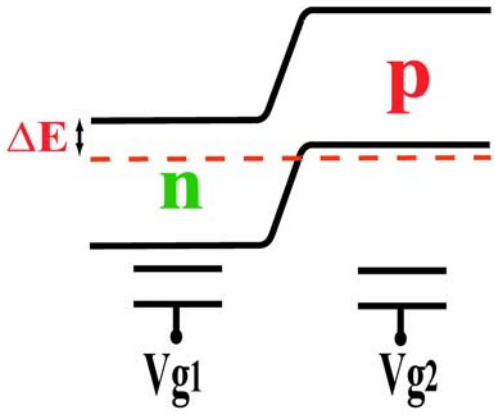
SUPPORTING INFORMATION

A. Simulated *I-V* characteristics of the carbon nanotube tunneling junction under reverse bias voltage

a



b

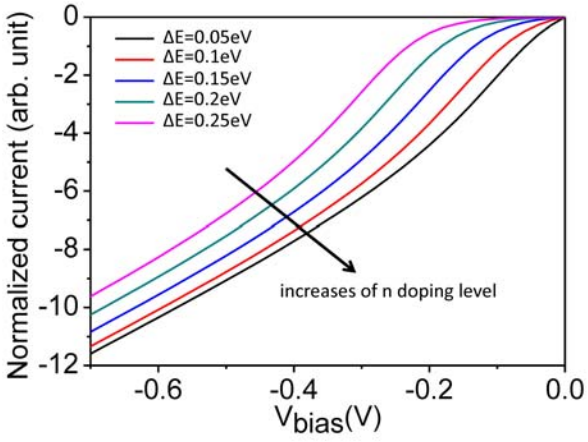


Figure S1 a, Energy band diagram under equilibrium with fixed degenerated p doping and varying n doping, represented by changes in ΔE. **b,** Simulated band-to-band tunneling in the reverse bias region.

Fig. S1(a) depicts band diagram under different equilibrium conditions. Fermi-level is initially near the band edge of the p side, and by changing V_{g1} gate voltage, doping level in the n side (ΔE) can be modulated. To numerically model *I-V* characteristics under the reverse bias voltage, Fermi's golden rule is employed to calculate the band-to-band tunneling current[1]:

$$I_{tunneling} \alpha \int_{E_{cn}}^{E_{vp}} \left(F_c(E) - F_v(E)\right) T N_c(E) N_v(E) dE$$

Here, $F_c(E)$ and $F_v(E)$ are Fermi-Dirac distribution functions at room temperature, and T is the tunneling probability through the junction potential barrier. $N_c(E)$ and $N_v(E)$ are density-of-states (DOS) of carbon nanotube for the conduction band and valence band, respectively. A large number of electronic states are near the band edge due to van Hove singularities. The equation integrates from the conduction band edge in the n side (E_{cn}) to the valence band edge in the p side (E_{vp}). From the equation, it is obvious that tunneling current is mainly decided by the overlap integral of DOS ($\int N_c(E) N_v(E)$), modulated by Fermi energy difference ($\int F_c(E) - F_v(E)$) between p and n side. For simplicity, only interband tunneling within the first subband is taken into consideration. Tunneling within higher subbands is negligible due to relative low tunneling probability[2]. The simulation results are plotted in the Fig. S1(b). Each curve shows similar *I-V* characteristics, with a nearly exponential current increase due to a large of DOS at van Hove singularity, and then followed by linear dependence under reverse bias voltage. In addition, *I-V* curve shifts toward downward direction by increasing doping level in the n side, which shows the same dependence as our experimental curves in the Fig. 3a. This theoretical simulation provides quantitative and predictive understanding of SWNT tunneling junction.

References for Supplementary Information

1 S. M. Sze, and K. K. Nq, Physics of Semiconductor Devices, Wiley, New York, 2006.

2 Jena, D.; Fang, T.; Zhang, Q.; Xing, H. L. Appl. Phys. Lett. **2008**, 93, 112106.