

Supplementary Information

1. Experimental detail:

The encapsulation procedure of iodine into SWNTs is as follows. First, SWNTs and iodine were set in two sub-tubes of a glass ampoule, and the ampoule was evacuated to 1×10^{-4} Pa (Fig. S1). Then the sub-tube with SWNTs was heated at 300 °C for 2 hours to eliminate the adsorbed gases; meanwhile, the other sub-tube with iodine was cooled by liquid nitrogen to avoid sublimation. Subsequently, the ampoule was sealed and heated at 150 °C for 48 hours in a furnace.

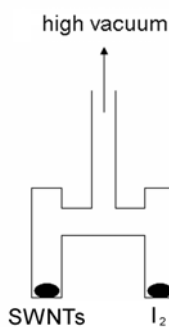


Figure S1. Schematic diagram of the apparatus.

2. Raman spectra:

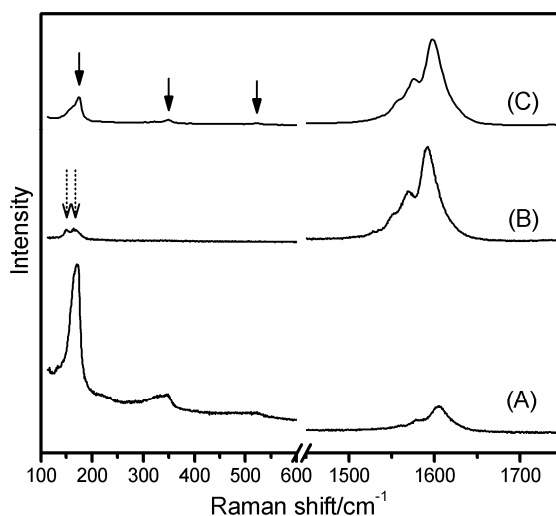


Figure S2. Raman spectra for I-SWNTs heated to 30 °C (A), 190 °C (B) and cooled to 30 °C from 190 °C (C). The solid and dotted arrows indicate the Raman peaks from charged polyiodide chains and SWNTs, respectively.

3. Calculation methods:

Vibrational properties are calculated by using the density functional theory (DFT) at the B3LYP¹ level using LanL2DZ² effective core basis set as implemented in the Gaussian 03 package³. For I₂, I₅, and I₇ confined in metallic (8, 8) and semiconducting (14, 0) SWNTs, geometry optimization and Mulliken analysis are carried out by using the SIESTA code⁴ based on generalized gradient approximation (GGA)⁵.

References

- (1) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1998, **37**, 785.
- (2) P. J. Hay and W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 270.
- (3) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian 03, Revision B.05; Gaussian, Inc., Wallingford CT, 2004.
- (4) J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon and D. Sanchez-Portal, *J. Phys. Condes. Matter* 2002, **14**, 2745.
- (5) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865.