

Supporting On-Line Material for:
Selective Probe of the Morphology and
Local Vibrations at Carbon Nanoasperities

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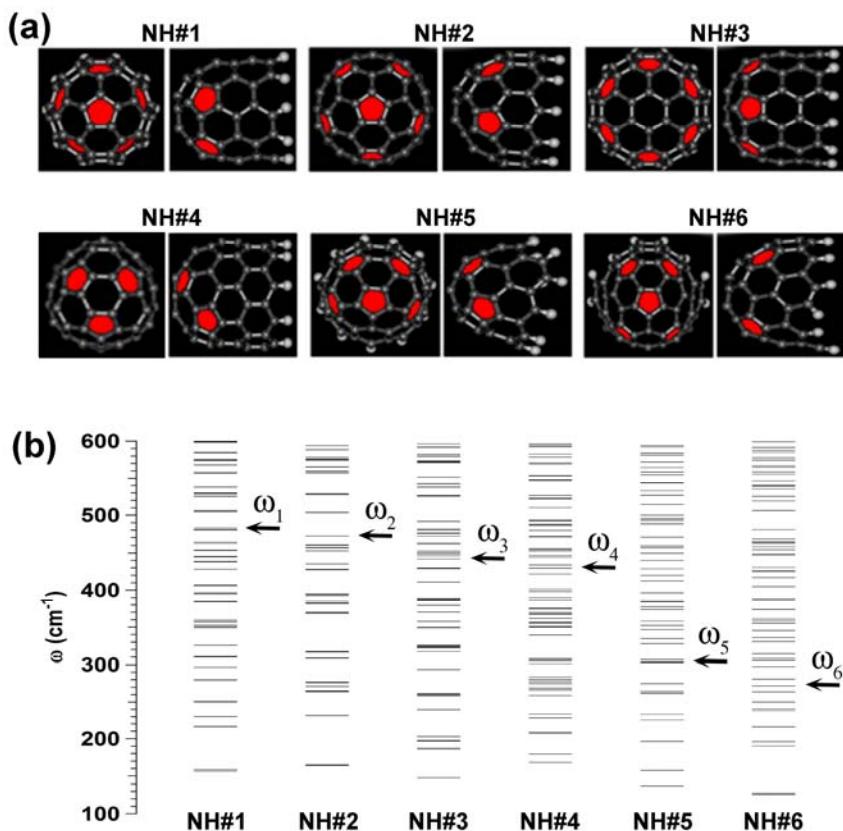


FIG. S1. (Color online) (a) Structural models used in the interpretation of vibrational modes of single-wall carbon nanohorns in top and side view. Structures NH#1-NH#4 represent nanohorn tips terminated by a short single-wall nanotube segment with a cap containing six pentagons. Structures NH#5 and NH#6 are nanohorns with five pentagons at the terminating cap. Pentagonal rings are highlighted in red for easy identification. Exposed edges of the finite-size structures are terminated by hydrogen atoms, shown by the white spheres. (b) Raman-active vibration modes of nanohorn structures NH#1-NH#6. Frequencies of the radial breathing mode and related modes expected to dominate the SERS spectrum are highlighted.

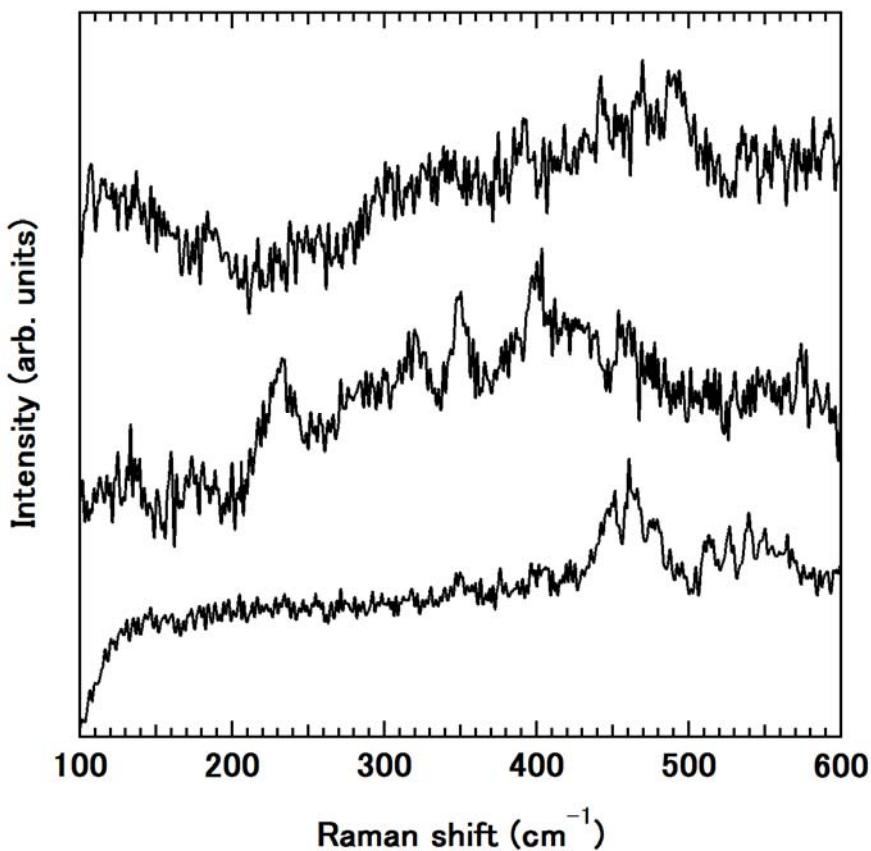


FIG. S2. SERS spectra of SWCNHs obtained at three different positions in the initial stage of SERS measurements.

Complete author list of Reference 14:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, T. Vreven, Jr., 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, 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 (2004), Gaussian 03, Revision C.02 and Gaussian, Inc.: Wallingford CT.