

Supporting Information: Details of the Transition Energy Model

The equations upon which the model is based on were reported by Strano *et al* [1]. In their approach the transition energies of metallic nanotubes are modelled as the transition energies of metallic armchair (n,n) tubes modified to take account of trigonal warping. Similarly the semiconducting nanotube transition energies are the transition energies of metallic armchair nanotubes scaled by the folding of the graphene dispersion relation and then again modified by the trigonal warping.

The model begins with an equation for the energy of a transition $v_i \rightarrow c_i$ for metallic armchair nanotubes :

$$\frac{1}{\lambda_{ii}^{armchair}} = \frac{A_{ii}}{hc} \left(\frac{d}{6\xi_{ii}a_{c-c}} + \frac{a_{c-c}B_{ii}}{4d} \right)^{-1} \quad (1)$$

where h and c are Plank's constant and the speed of light respectively, a_{c-c} is the carbon-carbon bond length and d is the diameter of the nanotube. A_{ii} and B_{ii} are transition dependent model parameters and ξ_{ii} is the scaling factor. The split bands of metallic nanotubes can be modelled as positive $\frac{1}{\lambda_{ii}^+}$ and negative $\frac{1}{\lambda_{ii}^-}$ deviations of equation 1 scaled by $\cos(3\alpha)^\tau$ where α is the chiral angle and τ is an integer.

$$\frac{1}{\lambda_{ii}^\pm} = \frac{1}{\lambda_{ii}^{armchair}} + \frac{2\beta_{ii}}{hc} \left(\mp \frac{3}{2} \left(\frac{a_{c-c}}{d} \right)^2 + 3\delta_{ii} \left(\frac{a_{c-c}}{d} \right)^3 \right) \cos(3\alpha)^\tau \quad (2)$$

where β_{ii} and δ_{ii} are again transition dependent model parameters.

For a metallic nanotube transition $v_1 \rightarrow c_1$ equation 2 uses :

$\xi_{11} = 1$ and	$\tau = 1$ for the positive deviation
	$\tau = 2$ for the negative deviation

For the semiconducting armchair nanotubes :

$$\frac{1}{\lambda_{ii}^{\pm}} = \frac{1}{\lambda_{ii}^{armchair}} + \frac{2\beta_{ii}}{hc} \left(\pm \frac{3}{2} \left(\frac{a_{C-C}}{d} \right)^2 + 3\delta_{ii} \left(\frac{a_{C-C}}{d} \right)^3 \right) \cos(3\alpha)^{\tau} \quad (3)$$

For a semiconducting nanotube transitions equation 3 uses :

$v_1 \rightarrow c_1$	$\xi_{11} = \frac{1}{3}, \tau = 1$
$v_2 \rightarrow c_2$	$\xi_{22} = \frac{2}{3}, \tau = 1$
$v_3 \rightarrow c_3$	$\xi_{33} = \frac{4}{3}, \tau = 1$

It is important to note that for a semiconducting nanotube transition $v_i \rightarrow c_i$ where i is odd the positive deviation represents a nanotube species where $mod\ 3\ (n - m) = -1$ and the negative root represents a species where $mod\ 3\ (n - m) = +1$. For transitions where i is even this correspondence is reversed

Model Parameters

For a metallic nanotube transition $v_1 \rightarrow c_1$:

A_{11}	3.2
B_{11}	4.47
β_{11}	4.1
δ_{11}	-0.48

For a semiconducting nanotube transitions :

$v_1 \rightarrow c_1$		$v_2 \rightarrow c_2$		$v_3 \rightarrow c_3$	
A_{11}	3.59	A_{22}	3.285	A_{33}	3.25
B_{11}	4	B_{22}	4.8	B_{33}	4.2
β_{11}	0.9	β_{22}	2.8	β_{33}	4.7
δ_{11}	-1.062	δ_{22}	-0.2	δ_{33}	-0.82

Comparison to Strano *et al*

The equations detailed above were fitted using the experimental data of Strano *et al* [1], it was then refined using the resonant Raman map of Telg *et al* [2] to produce a better fit. For comparison a summary of the fitting parameters published by Strano *et al* is repeated here.

For a metallic nanotube transition $v_1 \rightarrow c_1$:

A_{11}	3.0
B_{11}	4.47
β_{11}	2.23
δ_{11}	-0.78

For a semiconducting nanotube transitions :

$v_1 \rightarrow c_1$		$v_2 \rightarrow c_2$	
A_{11}	3.73	A_{22}	3.33
B_{11}	1.63	B_{22}	3.28
β_{11}	1.07	β_{22}	2.77
δ_{11}	-1.62	δ_{22}	-0.52

[1] M. S. Strano, S. K. Doorn, E. H. Haroz, C. Kittrell, R. H. Hauge and R. E. Smalley, Nano. Lett. **3**, 1091-1096 (2003)

[2] H. Telg, J. Maultzsch, S. Reich, F. Hennrich, and C. Thomsen, Phys. Rev. Lett. **93**, 177401 (2004)