

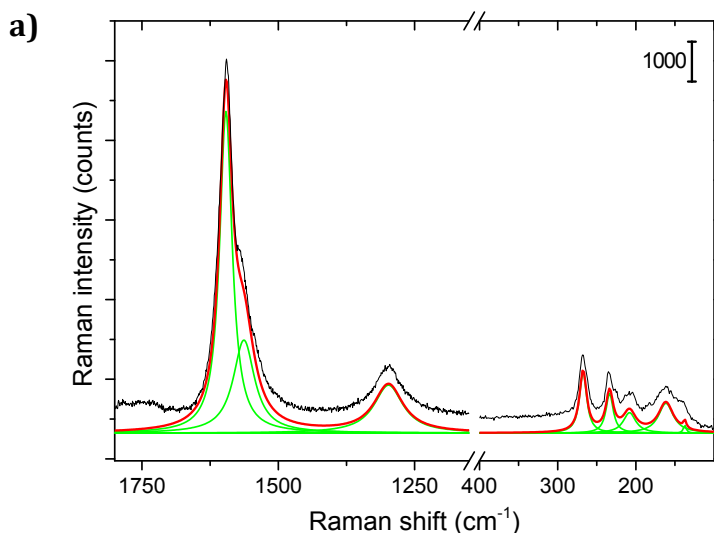
# Resonance Raman and IR spectroscopy of Aligned Carbon Nanotube Arrays with Extremely Narrow Diameters Prepared with Molecular Catalysts on Steel Substrates

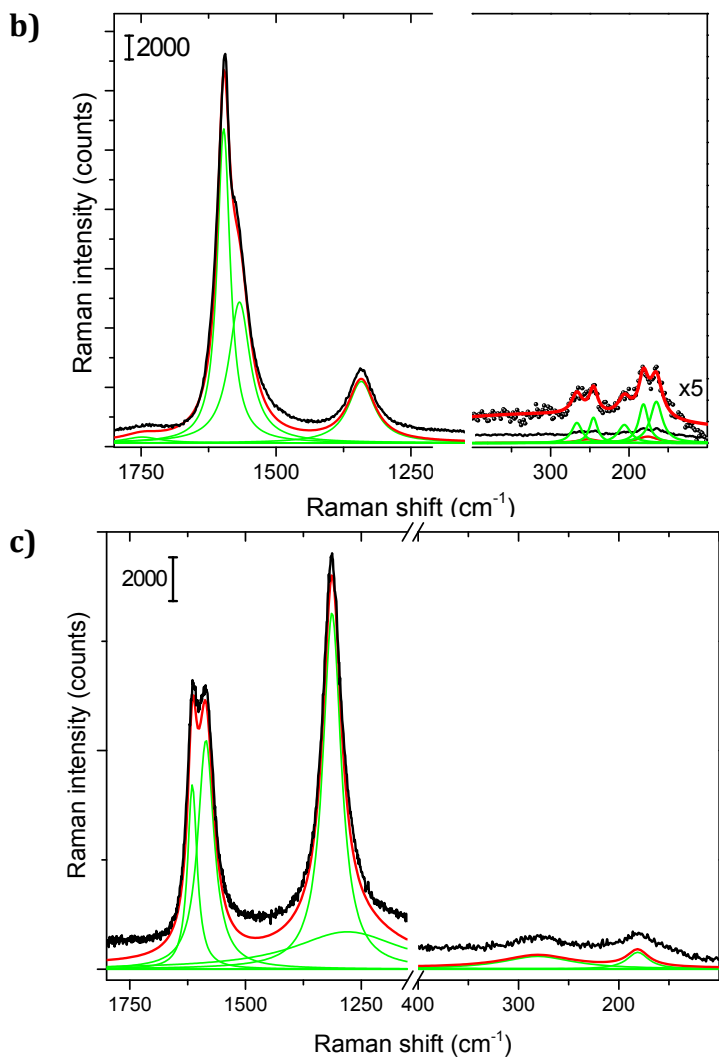
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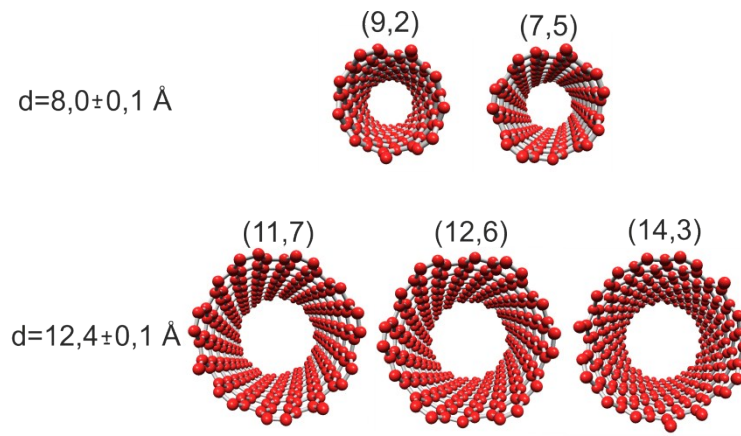
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## Electronic Supplementary Information (ESI)

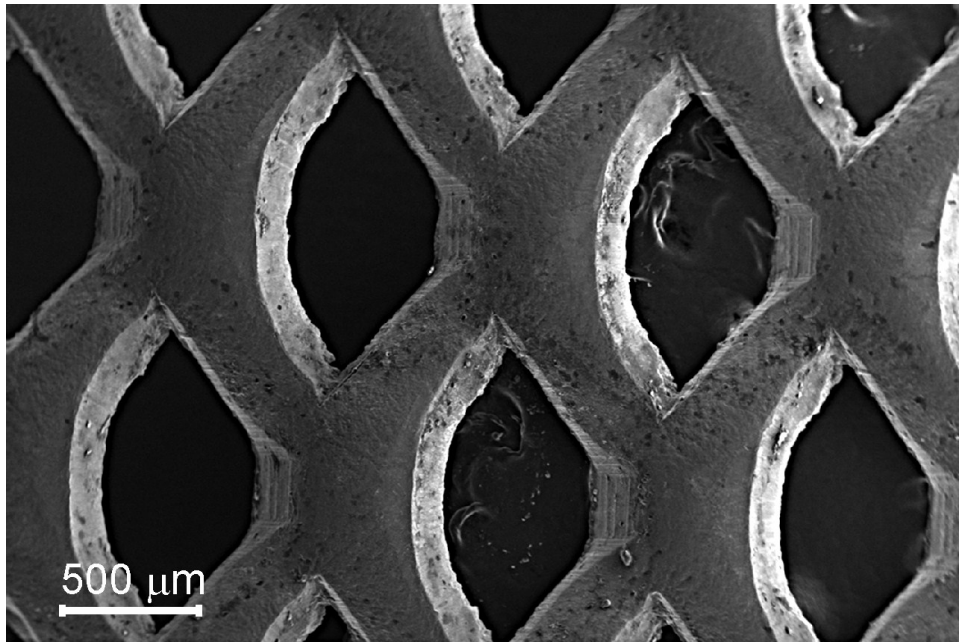




**Fig. S1.** First-order and radial-breathing-mode (RBM) Raman spectra of SWCNTs: a) and b) commercial (Elicarb) excited under 785nm and 514 nm laser lines, respectively, as compared to the as c) grown sample, excited under 785 nm laser line. Fittings of the simulated contributions as sum (red curves) and individual bands (green curves) are shown where the fit under the G<sup>-</sup> peak is best performed using a Lorentzian shape.



**Fig. S2.** Models of semiconducting SWCNTs with  $d = 8,0 \pm 0,1 \text{ \AA}$  and  $d= 12,4 \pm 0,1 \text{ \AA}$  corresponding to the maxima observed in the RBM region of the Raman spectra for the CNT grown on the grid ( $279.4 \text{ cm}^{-1}$  and  $180.4 \text{ cm}^{-1}$ ).



**Fig. S3.** SEM image of the steel grid used as a support.

**Table S1.** Chiral vector ( $C_k$ ), angle and diameter of the lowest and highest dimensional SWCNTs grown on the steel grids as extracted from analysis of the Raman spectra irrespectively of the G- line shape analysis.

CNT	$C_k$ (m,n)	Chiral angle <sup>a</sup> , ⊠ (degrees)	Diameter (nm)	Metallicity <sup>b</sup>	Band gap <sup>c</sup> (eV)
SWCNT	(9,2)	9.8	0.81	S	1.05
	(7,5)	24.5	0.83	S	1.02
	(8,4)	19.1	0.84	S	1.01
	(10,1)	8.4	0.84	M	-
	(11,7)	22.7	1.25	S	0.68
	(14,3)	9.5	1.25	M	-
	(12,6)	19.1	1.26	S	0.67

<sup>a</sup> Chiral angle as defined from the deviation from the zigzag direction ( $n=0$ , Fig 1 (a))

<sup>b</sup> Semiconducting (S) and metallic (M)

<sup>c</sup> Estimated through the parametrized equation  $E_g=(0.85 \text{ eVnm})/\text{diameter}$  and neglecting strain.

Table S2 Comparison of laboratory synthesis costs of CNTs and that from commercial companies.

CNTs	Price (\$/g)	Reference
SWCNTs	110	Thomas Swan Elicarb <a href="http://www.thomas-swan.co.uk/">http://www.thomas-swan.co.uk/</a>
MWCNTs	80	Mitsui <a href="https://www.mitsui.com/eu/en/index.html">https://www.mitsui.com/eu/en/index.html</a>
SWCNTs + MWCNTs	~ 35	This study