

Supporting Information for *Differentiation of Complex Vapor Mixtures Using Versatile DNA-Carbon Nanotube Chemical Sensor Arrays,*

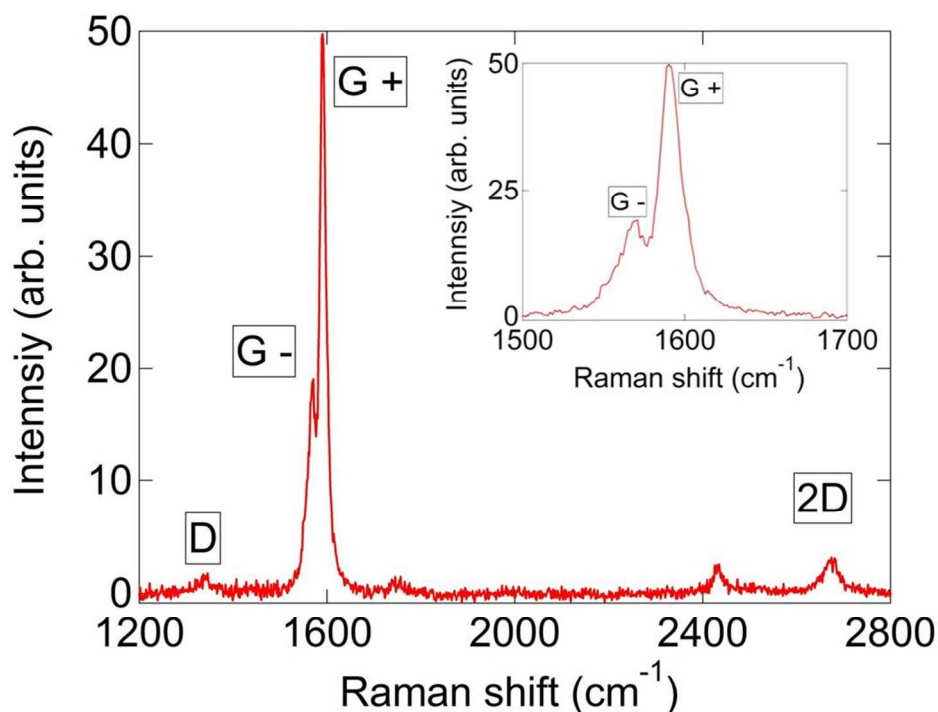
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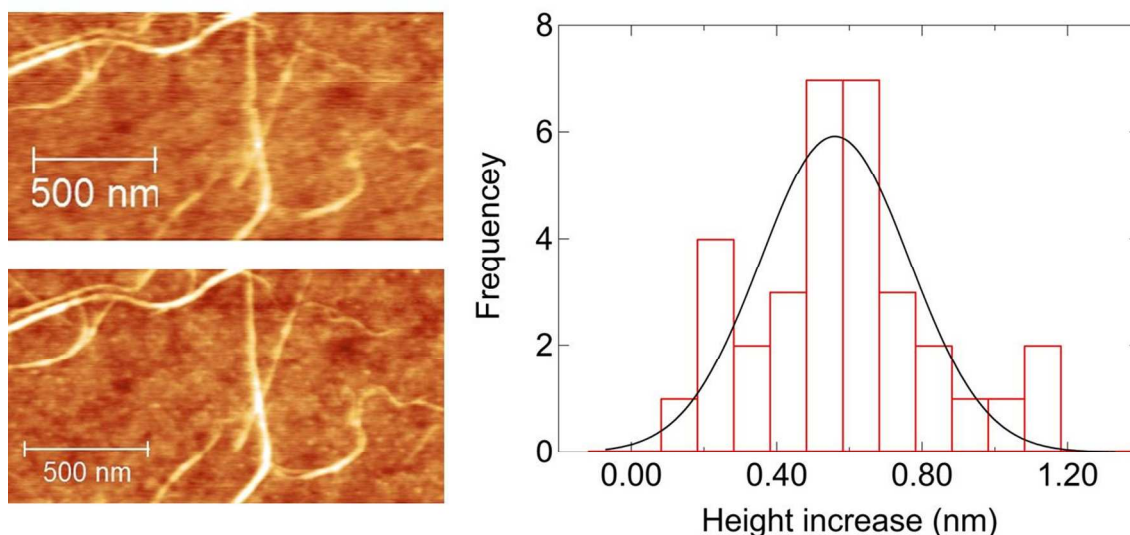
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Supplemental Figure 1: Raman spectrum of a carbon nanotube film deposited using the methods described in the main text. The very high G to D ratio (~ 50) indicates low defect density. The sharp G- peak, with FWHM similar to that of G+ peak, indicates that the sample contains a very high fraction of semiconducting nanotubes.¹



Supplemental Figure 2: AFM images of the same region before (left, top) and after (left, bottom) DNA functionalization. Thirty-three line scans were taken across matching locations in the two images, and the height of the as-deposited nanotube was compared to that of the same nanotube after DNA functionalization. There was a reproducible increase in the height of the nanotubes of 0.56 ± 0.2 nm as shown in the histogram of the differences (right). The black line in the histogram is a fit to a Gaussian distribution with mean of 0.56 nm and standard deviation of 0.20 nm.

Supplemental Table 1: Langmuir-Hill Fit Parameters for DMSO2 and Isovaleric Acid

DMSO2					Isovaleric acid			
	Seq 1	Seq 2	Seq 3	Seq 4	Seq 1	Seq 2	Seq 3	Seq 4
n	0.92 ± 0.10	0.36 ± 0.33	1.18 ± 0.34	1.77 ± 0.33	1.14 ± 0.44	0.59 ± 0.19	1.13 ± 0.35	1.45 ± 0.35
K_d (ppm)	0.89 ± 0.22	57.8	0.54 ± 0.21	0.67 ± 0.09	22 ± 13	83.5 ± 173	30 ± 17	14.9 ± 3.5
A (%)	-4.32 ± 0.48	-2.84 ± 0.04	-4.7 ± 0.9	-12.8 ± 1.2	1.83 ± 0.58	2.0 ± 1.4	2.35 ± 0.76	3.62 ± 0.53
Z (%)	-0.01 ± 0.09	-0.01 ± 0.21	0.02 ± 0.26	-0.02 ± 0.42	0.13 ± 0.08	0.08 ± 0.05	0.32 ± 0.08	0.25 ± 0.14

Supplemental Table 2: Responses (% change in current) for analyte-DNA oligomer combinations tested at representative concentrations

Seq	DMSO ₂	Isovaleric acid	D(+)-Limonene		L(-)-Limonene		α(+)	α(-)	β(-) pinene
	900 ppb	20ppm	15 ppm	100 ppm	15 ppm	100 ppm	130 ppm	130 ppm	130 ppm
1	-2.3	1.1	0.3	1.7	0.3	-1.3	-1.4	-1.3	-1.2
2	-0.5	0.6	2.9	3.5	2.1	-1.9	-5.3	-4.3	-3.4
3	-3.1	1.1	1.3	1.5	0.7	-1.7	-3.1	-2.4	-1.5
4	-8.2	2.7	0.5	1.1	2	-0.6	-3.4	-3.1	-2.9

The error in the measured responses is $\pm 0.05\%$.

Supplemental Table 3: Sensor responses (% change in current) for “parent” and “spiked” mixtures at 3% and 33% of a saturated vapor for each DNA sequence.

Seq	Parent mixture		10x acetic acid		10x nonanal		10x stearic acid	
	3%	33%	3%	33%	3%	33%	3%	33%
1	-0.7	-4.1	N/A	N/A	-1.0	-3.6	-0.7	-3.8
2	-2	-5.5	N/A	N/A	-2.2	-5.2	-1.9	-4.8
3	-1.7	-7.3	N/A	N/A	-2.9	-7.4	-1.6	-5.8
4	-2.5	-7	-4.25	-5.46	-3.2	-6.9	-2.4	-5.7

The error in the measured responses is $\pm 0.05\%$. Color coding in the spiked analyte columns indicates whether spiking the mixture made the response more negative (green) or less negative.

References

1. Dresselhaus, M. S.; Dresselhaus, G.; Jorio, A.; Souza Filho, A. G.; Saito, R., Raman Spectroscopy on Isolated Single Wall Carbon Nanotubes. *Carbon* **2002**, *40*, 2043-2061.