Carbon Nanotube Formic Acid Sensors Using a Nickel Bis(*ortho*-diiminosemiquinonate) Selector

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General Considerations

Compounds **1** and **2** were synthesized as reported in the literature.[1] Single-walled CNTs were purchased from NanoC (UPT-200). All other chemicals, solvents, and analytes (reagent grade) were purchased from commercial suppliers and used without purification. Milligram-scale masses were measured with a Satorius M2P microbalance. ^{1}H NMR spectra were recorded on 300 MHz and 500 MHz Varian spectrometers and referenced vs. solvent residual signal (d^6-DMSO: 2.50 ppm). UV-Vis absorption spectra were recorded with a Cary 4000 UV-Vis-NIR spectrometer. For UV-Vis-NIR samples, after sonication with CNTs, the samples were filtered through a 0.2 µm PTFE filter to remove insoluble material (i.e. CNTs and any strongly adsorbed species). Raman spectra were recorded with a Horiba HR800 spectrometer on samples enclosed in a quartz cuvette with a small piece of cotton. To generate saturated formic acid vapor conditions (FA), a drop of formic acid was placed on the cotton and the cuvette was carefully capped. Optical microscopy was used to confirm no movement of the Raman sample between ambient air and FA recordings.

Device Preparation

Glass microscope slides were cleaned by immersion in piranha solution for 1 h, followed by sonication in ultrapure water (Milli-Q), sonication in isopropanol, and drying. The slides and a custom stainless steel mask (Stencil.com) were mounted on a substrate holder using screws, and then loaded into an electron-beam physical vapor deposition system (AJA International, ATC-2036). Ti (20 nm) and Au (200 nm) were deposited. Ti was used as the adhesion layer to prevent corrosion that can affect devices made using Cr instead. The resulting microscope slides each contain 14 working electrodes, each separated from a shared counter electrode by a 1 mm gap.

A vial containing 1 mg of CNTs in 4 mL of o-dichlorobenzene was bath-sonicated. Using a micropipette, 1 μL of this solution was placed on each of the 14 working/counter electrode gaps, and solvent was removed in a vacuum chamber to yield a conductive film. This vacuum dropcasting was repeated until each device exhibited a resistance of 1-10 kΩ as measured by a handheld multimeter (in most cases, 1-2 dropcastings achieves this resistance). To apply a selector, 1 μL of a DMF solution of the selector (1 mg/mL) was added to the CNT network and dried under vacuum. For consistency, CNT chemiresistors without added selectors were also treated with 1 μL of pure DMF and dried under vacuum.

Gas Detection Experiments

Analyte gas streams were generated with a KIN-TEK FlexStream gas generator. Unless otherwise noted, liquid analyte was placed in an uncapped (size 15-425) test tube in the analyte oven at 40 ^{o} C to generate vapors. The mass loss of the analyte sources over a set period of time was used to calculate emission rates (ng/min), which was then used to convert oven and diluent flow rates into analyte concentrations (ppm). For highly corrosive trifluoroacetic acid and dichloroacetic acid, no attempt to determine an emission rate, to protect against corrosion of the gas generator. Analyte streams were introduced to the sensor in a custom PTFE enclosure. A USB multiplexer (PalmSens) applied a 0.1 V bias across each device and measured the current as a function of time.

Lower concentrations of formic acid vapor were achieved without excessive diluent flow by construction of a permeation tube, as illustrated in Figure S3. A 1 dram glass vial with an open-faced screw cap (size 13-425) was filled with formic acid and covered with a 0.5” diameter disc cut from 0.001” thick PFA film (McMaster-Carr) and a PTFE o-ring before being screwed shut. To determine the emission rate of this device, the tube was placed in the analyte oven for 1 h (at 70 sccm oven flow, 40 ^{o} C oven temperature) and then an initial mass was recorded. The tube was then kept in the analyte oven for 8.5 days, and an emission rate of 707 ng/min was determined. For comparison, an uncapped (size 15-425) test tube of formic acid under the same oven conditions emits at 2.512 x 10^5 ng/min.

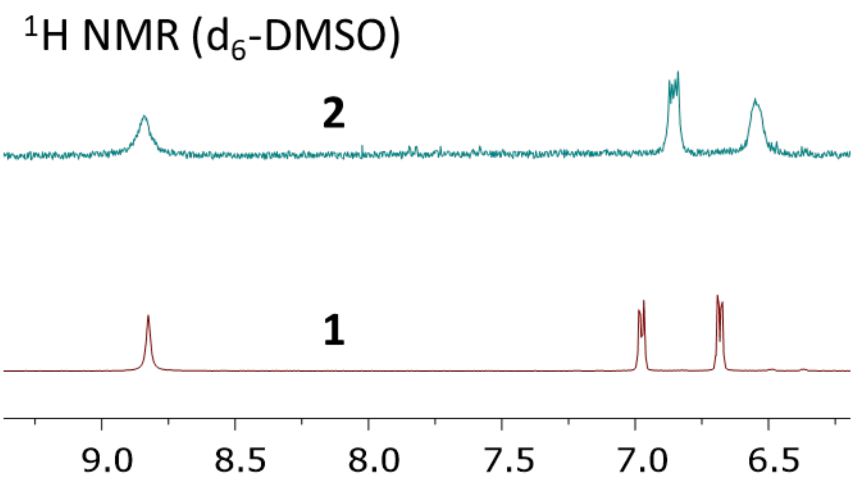

Figure S1. ^{1}H NMR spectra of **1** and **2**

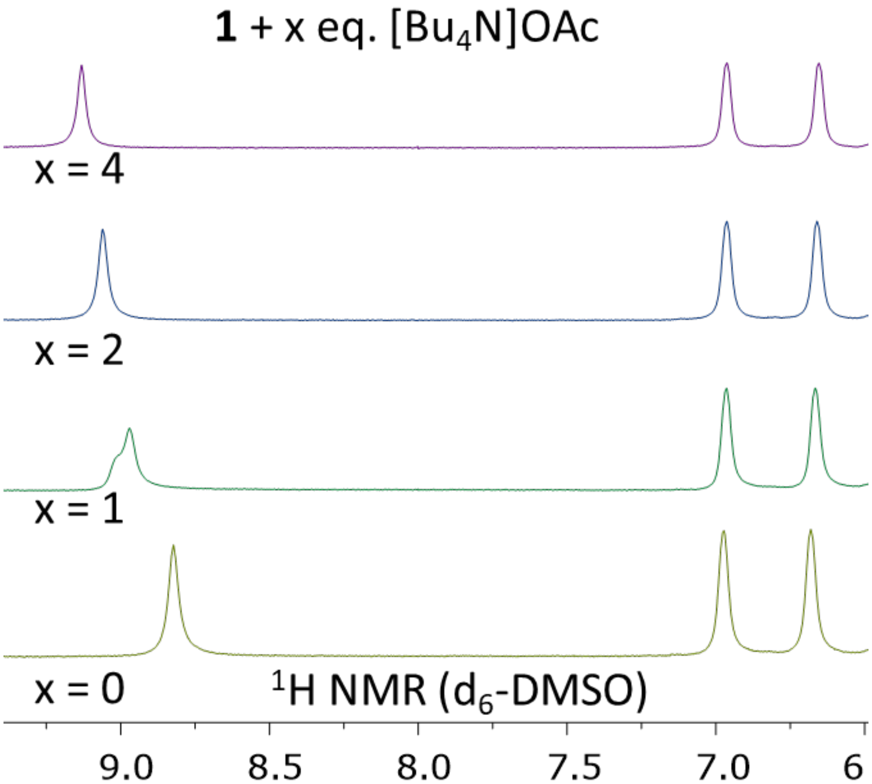

Figure S2. ^{1}H NMR spectra (300MHz) monitoring addition of $[Bu_4N]OAc$ to **1**

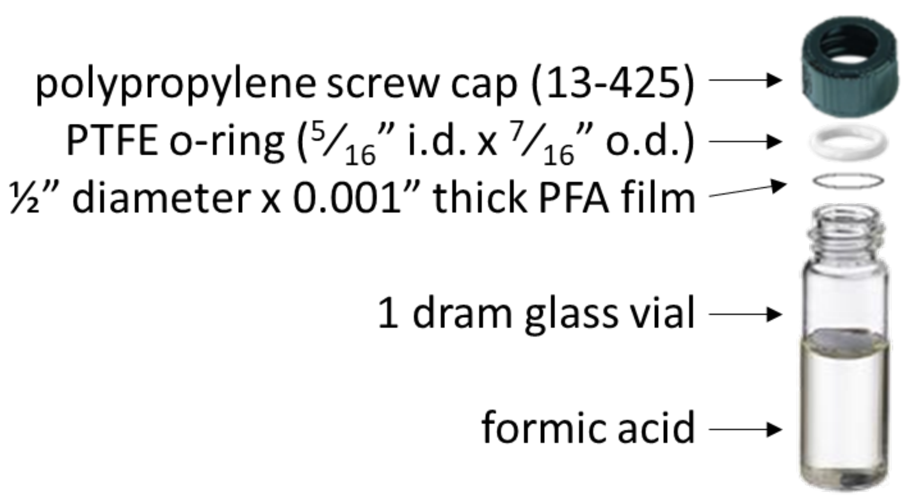

Figure S3. Construction of custom low-emission permeation tube

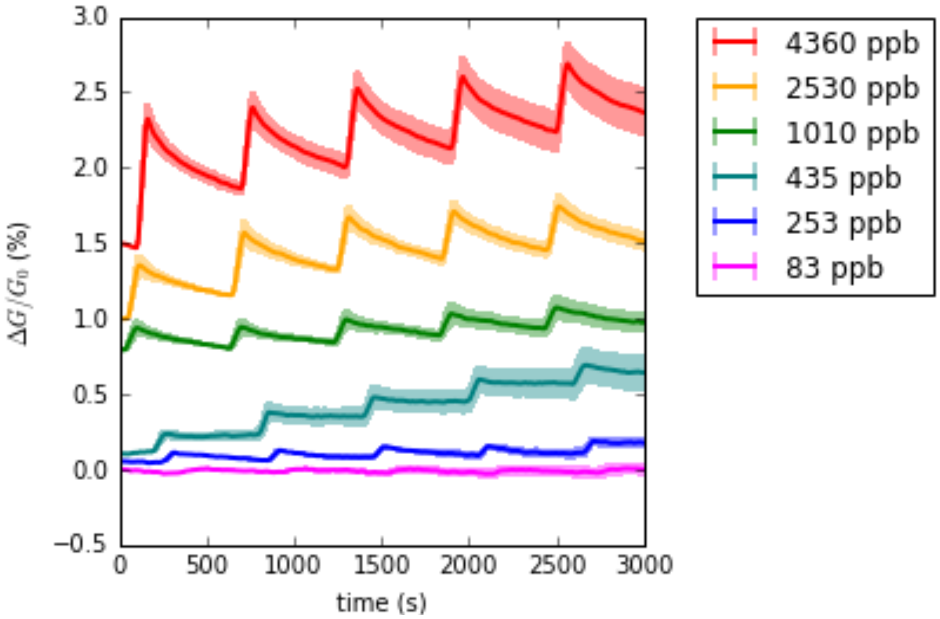

Figure S4. Average conductivity traces (*N*=4) of CNT/**1** upon exposure to various concentrations of formic acid vapor.

The one-minute exposure and nine-minute purge was cycled 5 times. These traces were used to plot the lower six concentration data points on Figure 3a in the main text.

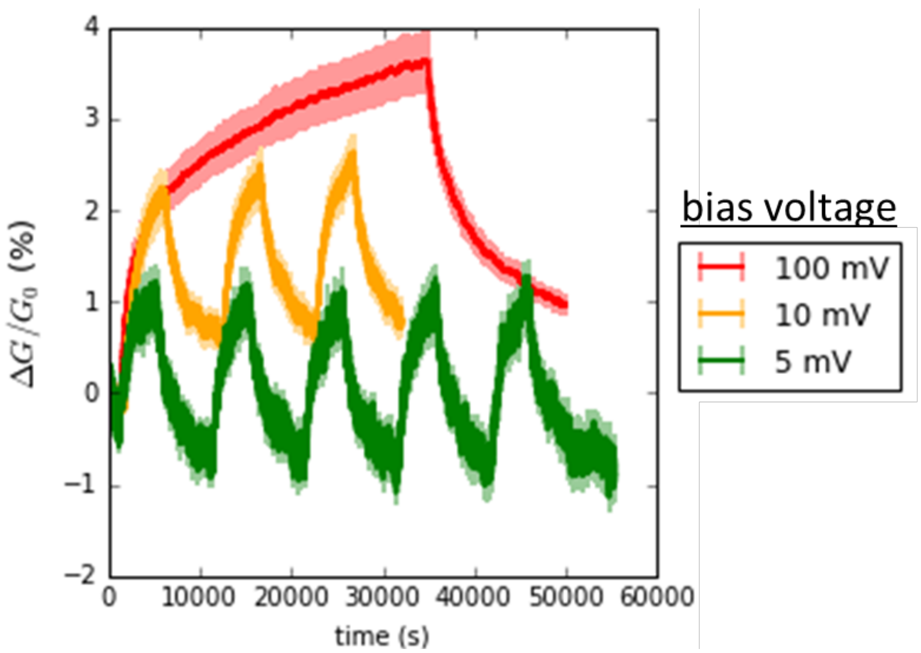

Figure S5. Longer formic exposures and effect of varying bias voltage.

The chemiresistive response to 3.7 ppm formic acid (0.2% of saturated vapor from 40 ^{o} C analyte oven) does not saturate with a 500 min exposure time, but most of the response happens in the beginning (red trace). Lowering the bias voltage yields noisier but similar responses with 50 minute exposures (red, orange, and green traces), supporting that this is a chemiresistive and not a fuel-cell sensor, which would yield lower responses with lower bias voltages.

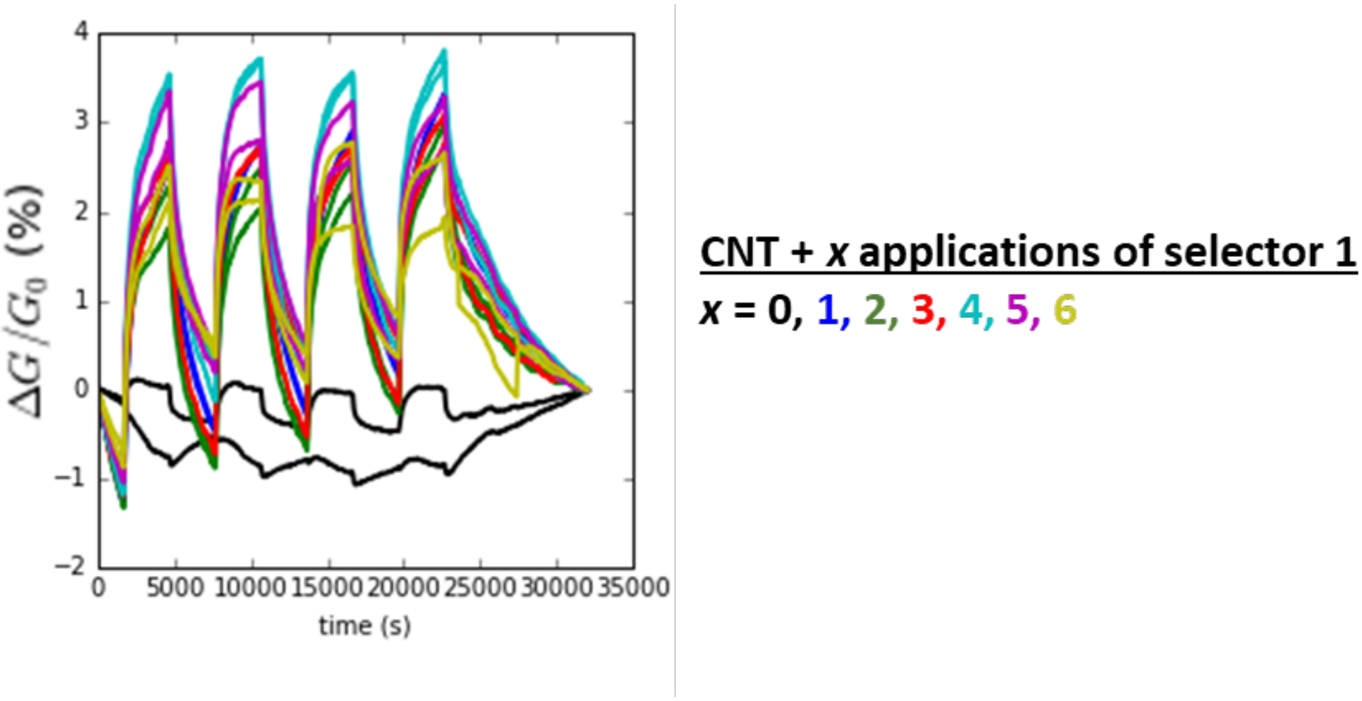

Figure S6. Changes in conductivity upon formic acid exposure (37 ppm) as an effect of loading of **1**.

Traces are color-coded by selector loading, with ***x*** 1 uL drops of 1 mg/mL **1**/DMF applied to the CNT network. The sensing enhancement between *x*=0 and *x*=1 was large, with minimal improvements in sensing for *x*=2–5. Over-loading of the selector (*x*=6) diminished sensor response.

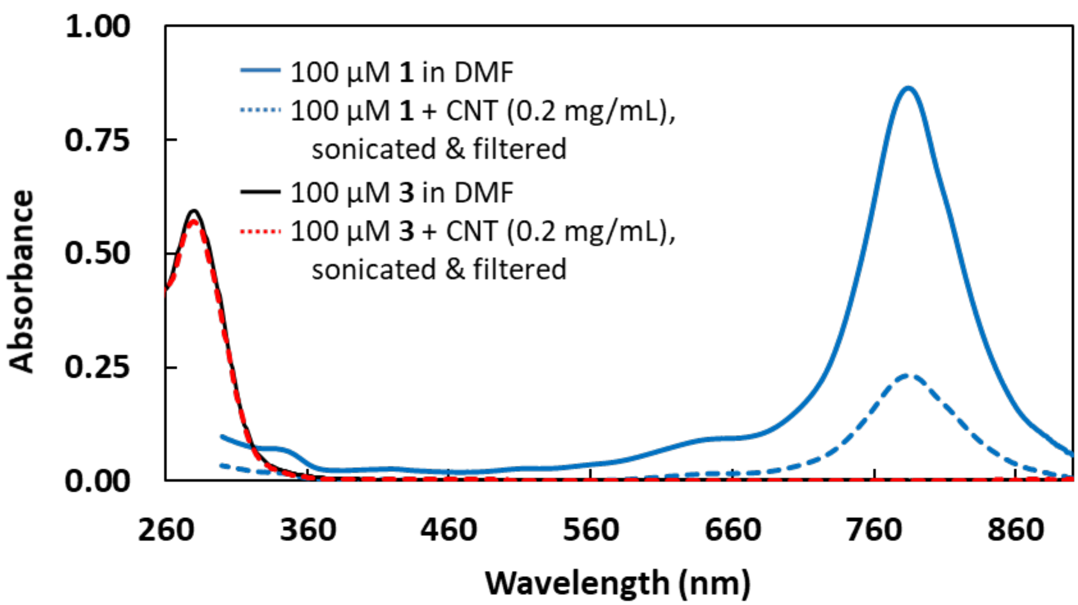

Figure S7. UV-Vis-NIR absorption spectrum of **1** and **3** in DMF before and after sonication with CNT and filtration.

The CNTs visibly remained mostly aggregated after 1 minute of bath sonication; filtration was performed to eliminate scattering effects.

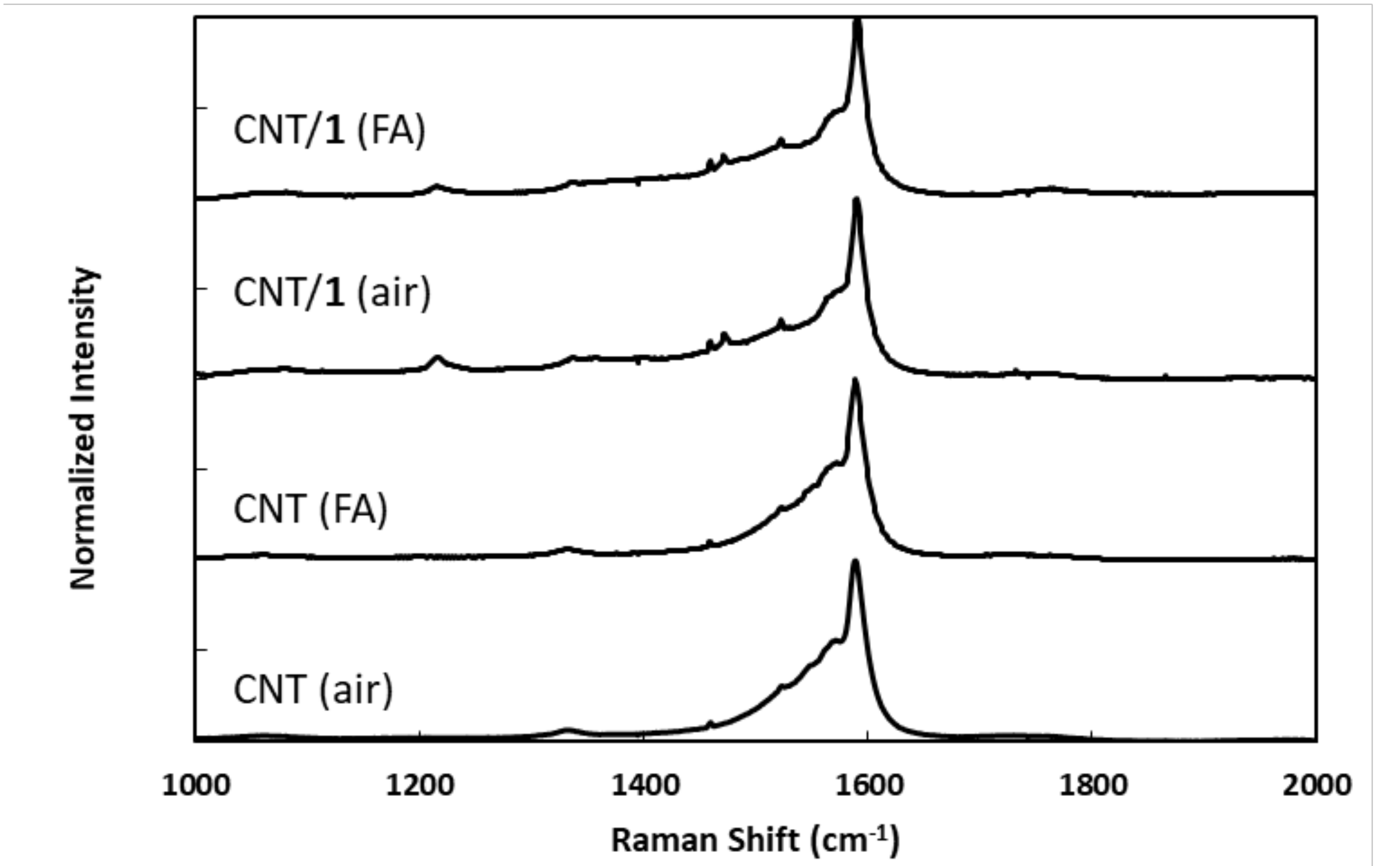

Figure S8. Raman spectra of sensing materials under ambient air or saturated formic acid vapor (FA).

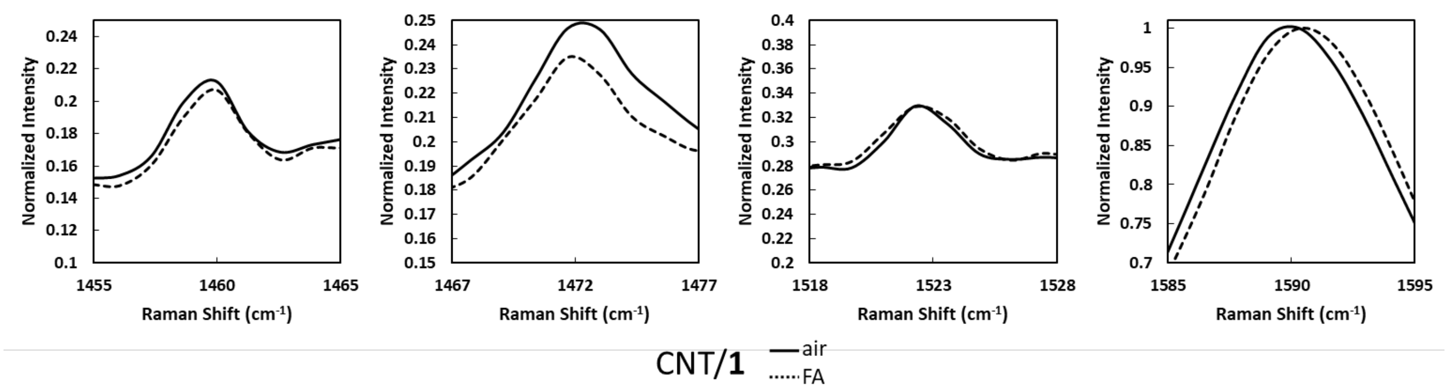

Figure S9. 10 cm^{-1}-wide windows of sharp features of Raman spectra of CNT/**1**.

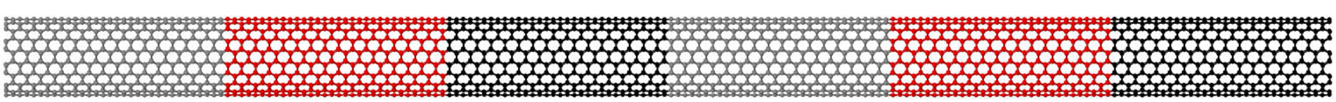

Figure S10. Visualization of 640 carbon segments in a (10,10)-CNT.

Each colored 640 carbon segment corresponds to the region for one protonation of CNT/**1** under saturated formic acid vapor, as determined by 0.5 cm^{-1} shift of the Raman spectrum G-band vs. ambient air recording.

Computational Details.

Initial nanotube coordinates were generated with the Nanotube Builder module of Avogadro.[3] Geometry optimizations were performed using the Gaussian 09.[4] The ONIOM partitioning schemes are shown in Figure S11 below. The high-level model was treated with DFT using the ωB97XD functional[5] (with built-in dispersion[5] and long-range corrections) and the 6-31G basis set,[6] while the low-level model was treated semiempirically with PM6.[7] Using the "scf=xqc" keyword assisted the calculations in converging. Optimized structures were then analyzed by a single-point calculation, with all atoms being treated by DFT as implemented in Orca v3.0.3[8] using the ωB97X-D3 functional, def2-SVP basis set,[9] and the RIJCOSX Resolution of Identity approximation. While these parameters could find a stable broken-symmetry electronic state for **1** alone (using the Flipspin and FinalMs keywords), (6,6)-CNT/**1** converged to a closed-shell solution. Multiwfn was used to translate the Orca calculation output into density-of-states plots and Fermi levels (Gaussian broadening, FWHM = 0.300 eV).[10]

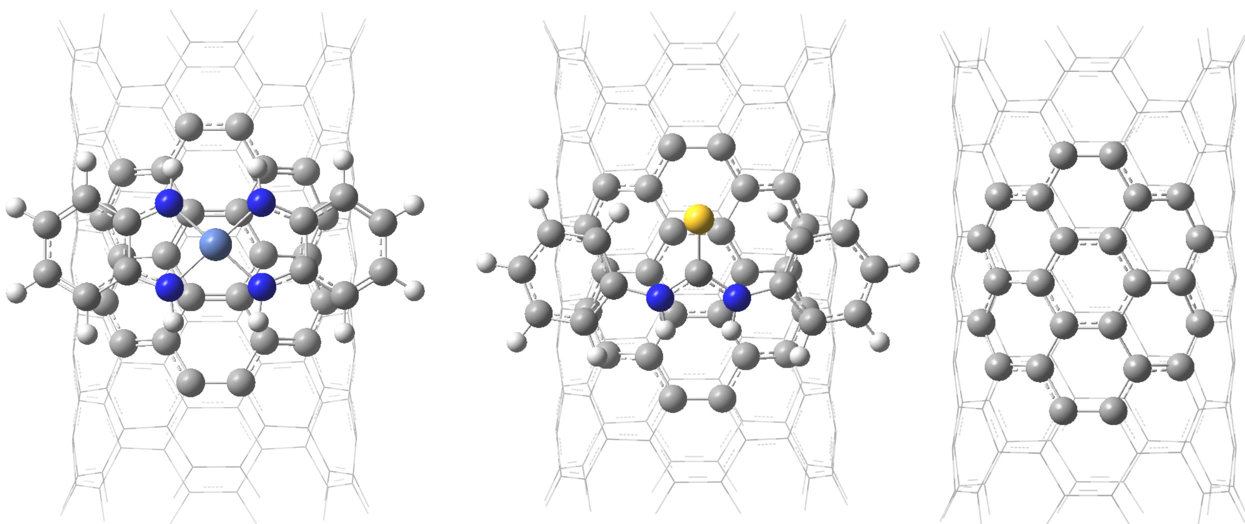

Figure S11. ONIOM-optimized structures

Left to right: (6,6)-CNT/**1**, (6,6)-CNT/**3**, and (6,6)-CNT. Ball-and-stick atoms assigned to the high-level model (DFT) and the wireframe portion assigned to the low-level model (PM6).

Table S1. Coordinates of (6,6)-CNT/**1**

C	4.956450	-0.260680	-4.086710
C	4.964750	-1.692980	-4.091150
C	3.741900	-2.371640	-3.878850
C	3.748920	-3.616470	-3.143580
C	4.977060	-4.118600	-2.650840
C	4.981640	-4.824380	-1.403110
C	3.757440	-4.980710	-0.712060
C	3.757060	-4.980670	0.733720
C	4.981780	-4.812600	1.422810
C	4.977610	-4.107360	2.670890
C	3.750010	-3.597560	3.154500
C	3.742000	-2.352750	3.889830
C	4.965100	-1.669690	4.090720
C	4.957240	-0.237040	4.087120
C	3.727470	0.430330	3.877000
C	3.719400	1.670660	3.136620
C	4.939910	2.183490	2.640240
C	4.932180	2.895850	1.400680
C	3.691240	3.065680	0.714250
C	3.690750	3.069390	-0.738040
C	4.932000	2.884330	-1.421870
C	4.939680	2.172960	-2.661400
C	3.719370	1.651810	-3.148810
C	3.726310	0.411280	-3.888540
C	2.484470	-0.283770	-4.069750
C	2.493790	-1.689690	-4.062460
C	1.243990	-2.398890	-3.882070
C	1.251520	-3.619560	-3.157690
C	2.506000	-4.103120	-2.619630
C	2.511230	-4.795840	-1.397120
C	1.259850	-4.999590	-0.698000
C	1.259970	-5.001550	0.720840
C	2.510910	-4.784420	1.416300
C	2.506980	-4.092460	2.639220
C	1.252030	-3.598920	3.167590
C	1.244600	-2.380130	3.894870
C	2.493850	-1.667110	4.061600
C	2.485890	-0.261320	4.069480
C	1.228280	0.437030	3.909280
C	1.218820	1.666910	3.176190
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C	2.463400	2.851750	1.406070
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C	1.202950	3.013980	-0.716060
C	2.462430	2.839360	-1.426120
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C	1.217990	1.646090	-3.187030
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C	-1.206710	-3.634190	-3.157450
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C	0.002890	-0.253720	4.122410
C	-1.230600	0.422500	3.909470
C	-1.235860	1.652550	3.176510
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C	-6.131850	-5.184340	0.695110
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C	-4.925770	-4.166350	2.671660
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C	-4.942080	-1.728570	4.091290
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C	-6.168080	0.475680	3.966980
C	-6.175430	1.647410	3.271310
C	-4.962890	2.124790	2.640930
C	-4.963750	2.837350	1.401420
C	-6.174710	3.125480	0.668750
C	-6.176440	3.126420	-0.693630
C	-4.963860	2.825940	-1.421130
C	-4.963330	2.114370	-2.660610
C	-6.174400	1.626240	-3.283860
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H	-7.063680	-2.150880	-4.420220
H	-7.047070	-4.306880	-3.157800
H	-7.044000	-5.366170	-1.234550
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H	-7.048590	-4.282220	3.168370
H	-7.061150	-2.131020	4.438970
H	-7.079700	0.071080	4.406350
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H	-7.089840	3.298060	-1.260080
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C	6.158120	1.720650	3.270580
C	6.164780	0.548980	3.966320
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C	6.195450	-5.110730	0.694100
C	6.193760	-5.111150	-0.669370
C	6.186820	-3.644420	-3.287750
C	6.179310	-2.469760	-3.979220
C	6.165820	0.527230	-3.979440
C	6.156340	1.699340	-3.284990
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H	7.064970	2.306170	3.134600
H	7.081180	0.155300	4.405700
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H	7.101720	-4.198040	3.167350
H	7.107990	-5.286070	1.260400
H	7.109390	-5.281670	-1.235710
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H	7.090170	-2.066850	-4.421770
H	7.078670	0.135810	-4.423850
H	7.066210	2.282900	-3.145690
H	7.052250	3.381660	-1.261170
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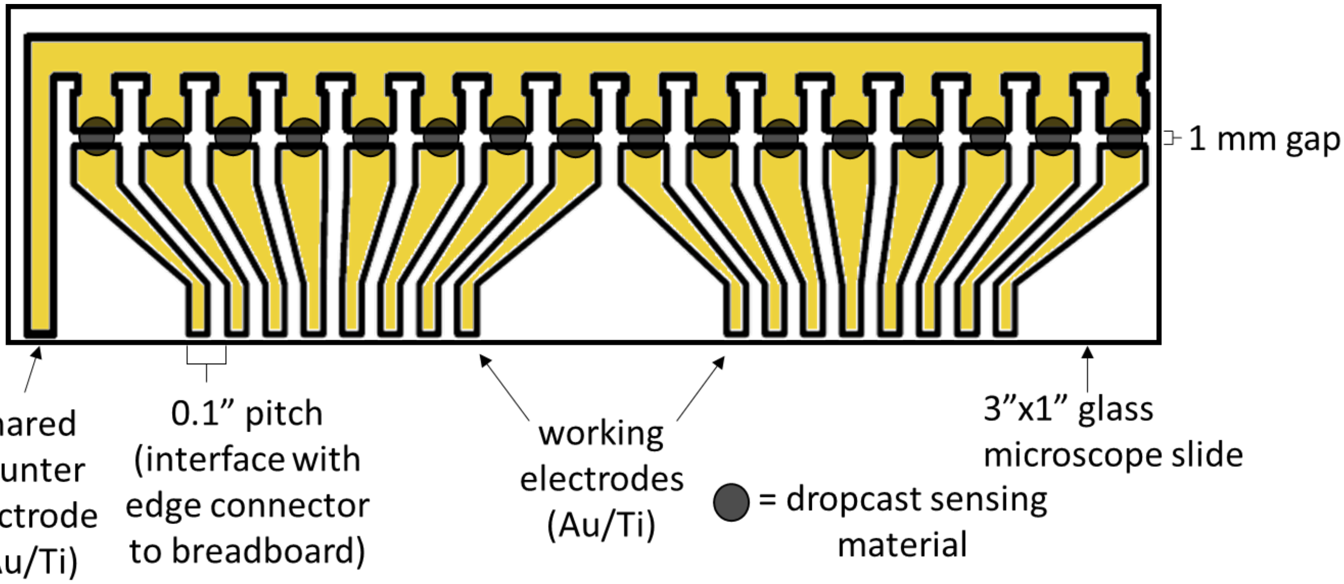
C	-1.459780	5.466160	-3.715180
C	-0.757140	5.844530	-2.546600
C	0.672790	5.852900	-2.547020
C	1.379050	5.481390	-3.715600
C	0.671380	5.111600	-4.839440
H	-1.276530	4.796050	-5.735270
H	-2.544870	5.441950	-3.706390
H	2.464340	5.469130	-3.707330
H	1.202370	4.808650	-5.735410
C	-0.755230	5.841670	2.546290
C	-1.456710	5.464000	3.715490
C	-0.744460	5.107450	4.840880
C	0.675220	5.118750	4.840940
C	1.381880	5.486740	3.715670
C	0.674590	5.852940	2.546310
H	-2.541730	5.436770	3.706580
H	-1.271620	4.800260	5.737650
H	1.207110	4.820270	5.737870
H	2.467190	5.477550	3.707150
N	-1.266010	6.159670	-1.332960
N	1.178580	6.175050	-1.333860
N	1.179620	6.173510	1.332090
N	-1.265310	6.154820	1.332270
Ni	-0.044240	6.321120	-0.000480
H	2.184410	6.135710	-1.221710
H	-2.271290	6.108970	-1.220470
H	-2.270640	6.102820	1.220670
H	2.185720	6.138990	1.220770

Table S2. Coordinates of (6,6)-CNT/**3**

C	4.913173	-0.518916	-4.090898
C	4.806179	-1.947768	-4.098044
C	3.532905	-2.526130	-3.886880
C	3.439386	-3.767185	-3.151418
C	4.623024	-4.366572	-2.658093
C	4.570133	-5.071030	-1.410517
C	3.337117	-5.128584	-0.719961
C	3.335778	-5.131624	0.725651
C	4.569829	-5.064877	1.415961
C	4.621441	-4.366666	2.666812
C	3.438426	-3.762028	3.152462
C	3.529586	-2.524369	3.893869
C	4.803824	-1.941651	4.096840
C	4.910613	-0.513474	4.098117
C	3.738069	0.250680	3.889777
C	3.828698	1.487491	3.149581
C	5.086521	1.900847	2.651654
C	5.135317	2.608641	1.411447
C	3.911705	2.875338	0.723948
C	3.912173	2.877170	-0.725083
C	5.136320	2.604571	-1.410481
C	5.088832	1.900860	-2.654506
C	3.831784	1.482318	-3.146080
C	3.740373	0.248805	-3.891973
C	2.447261	-0.343976	-4.077317
C	2.343370	-1.746224	-4.071739
C	1.041036	-2.352549	-3.892308
C	0.949965	-3.569669	-3.166858
C	2.161178	-4.152168	-2.627986
C	2.110034	-4.843374	-1.405468
C	0.846444	-4.946349	-0.707151
C	0.845480	-4.951608	0.711912
C	2.109222	-4.838215	1.408500
C	2.159913	-4.153405	2.634764
C	0.948701	-3.563465	3.165114
C	1.038327	-2.351925	3.899492
C	2.340604	-1.742142	4.069410
C	2.445091	-0.339790	4.082821
C	1.247827	0.456832	3.924985
C	1.336983	1.683630	3.191018
C	2.615556	2.077241	2.638792
C	2.671443	2.759452	1.416082
C	1.429589	3.022078	0.704567
C	1.429752	3.026023	-0.707390
C	2.672493	2.755727	-1.416681
C	2.618355	2.078270	-2.642505
C	1.339753	1.677022	-3.187300
C	1.250574	0.456355	-3.932511
C	-0.025941	-0.136766	-4.132373
C	-0.133955	-1.580894	-4.117735
C	-1.410419	-2.170053	-3.893309
C	-1.501700	-3.386423	-3.167800
C	-0.313703	-3.986591	-2.665089
C	-0.367493	-4.699078	-1.407619
C	-1.604908	-4.763235	-0.707930
C	-1.605838	-4.768666	0.710988
C	-0.367859	-4.693760	1.407841
C	-0.315896	-3.989554	2.669978
C	-1.503356	-3.381457	3.164821
C	-1.413297	-2.170112	3.899789
C	-0.136671	-1.578165	4.112677
C	-0.029493	-0.134292	4.137078
C	-1.205379	0.638247	3.926065
C	-1.112282	1.864203	3.191486
C	0.148648	2.254465	2.679318
C	0.200566	2.945890	1.400357
C	-1.004741	3.187073	0.703300
C	-1.003947	3.198333	-0.707712
C	0.202613	2.941767	-1.400888
C	0.151059	2.254333	-2.680935
C	-1.109392	1.856970	-3.188203
C	-1.202272	0.638658	-3.934096
C	-2.504005	0.024489	-4.081661
C	-2.609212	-1.377664	-4.075047
C	-3.900774	-1.972817	-3.891012
C	-3.992855	-3.213415	-3.154529
C	-2.786079	-3.783127	-2.629893
C	-2.839060	-4.473819	-1.407120
C	-4.095057	-4.573645	-0.722488
C	-4.095337	-4.577302	0.723128
C	-2.838938	-4.469372	1.406891
C	-2.788463	-3.785434	2.633575
C	-3.995278	-3.210071	3.151225
C	-3.903063	-1.973246	3.894002
C	-2.610940	-1.375131	4.070100
C	-2.507499	0.027233	4.084604
C	-3.699528	0.801402	3.891915
C	-3.607010	2.037897	3.151122
C	-2.318258	2.439698	2.641115
C	-2.272768	3.122245	1.416718
C	-3.482974	3.419338	0.722885
C	-3.481242	3.428126	-0.729119
C	-2.271913	3.115774	-1.419157
C	-2.317297	2.442698	-2.647079
C	-3.605442	2.034429	-3.151801
C	-3.695993	0.801688	-3.898380
C	-4.969300	0.215301	-4.097178
C	-5.075012	-1.212510	-4.103633
C	-6.339570	-1.905227	-3.992411
C	-6.427085	-3.075973	-3.300036
C	-5.252541	-3.630364	-2.661657
C	-5.305736	-4.333713	-1.413854
C	-6.534663	-4.538026	-0.680809
C	-6.536897	-4.541131	0.682762
C	-5.306154	-4.329413	1.412736
C	-5.254568	-3.632662	2.664727
C	-6.426971	-3.070812	3.297005
C	-6.343173	-1.902687	3.994995
C	-5.077258	-1.210009	4.098279
C	-4.972113	0.219182	4.099649
C	-6.122924	1.085302	3.977258
C	-6.036177	2.253874	3.280896
C	-4.789080	2.631738	2.651552
C	-4.731866	3.340048	1.410047
C	-5.914733	3.725168	0.676506
C	-5.915761	3.729556	-0.686100
C	-4.731702	3.334809	-1.415047
C	-4.787123	2.634827	-2.659735
C	-6.033164	2.249031	-3.286390
C	-6.122140	1.084045	-3.986849
H	-7.220577	-1.442045	-4.436454
H	-7.376751	-3.591562	-3.172121
H	-7.459888	-4.643754	-1.247528
H	-7.459755	-4.655138	1.248085
H	-7.380105	-3.581760	3.160468
H	-7.221715	-1.444242	4.444172
H	-7.064924	0.754700	4.414896
H	-6.901512	2.898799	3.143247
H	-6.816111	3.963017	1.242485
H	-6.812827	3.975336	-1.251633
H	-6.901014	2.892864	-3.144298
H	-7.059172	0.758066	-4.433956
C	6.365260	2.822731	-0.682384
C	6.362634	2.820873	0.680268
C	6.263913	1.342860	3.283479
C	6.177260	0.174371	3.978653
C	5.953682	-2.814341	3.994699
C	5.864201	-3.982934	3.298722
C	5.755843	-5.457726	0.686873
C	5.754792	-5.455178	-0.676685
C	5.867106	-3.991073	-3.294082
C	5.954281	-2.819290	-3.985302
C	6.181238	0.168646	-3.979162
C	6.264327	1.334874	-3.278954
H	7.286950	2.932462	1.247766
H	7.213951	1.856268	3.148993
H	7.058916	-0.290866	4.419064
H	6.890273	-2.489558	4.443368
H	6.731253	-4.629452	3.163354
H	6.651315	-5.706789	1.252917
H	6.654358	-5.697226	-1.242920
H	6.730593	-4.640434	-3.164773
H	6.895145	-2.490322	-4.426498
H	7.060812	-0.292455	-4.423632
H	7.217892	1.843339	-3.135432
H	7.287264	2.942388	-1.248282
C	-0.696342	5.473194	-4.699719
C	-0.898477	5.825334	-3.370330
C	0.187483	5.942544	-2.487839
C	1.483928	5.715820	-2.962042
C	1.672744	5.367137	-4.299751
C	0.595246	5.239056	-5.174030
H	-1.549955	5.373696	-5.361437
H	-1.908874	5.990590	-3.005851
H	2.681608	5.179681	-4.651081
H	0.756977	4.956971	-6.208486
C	0.181283	5.945284	2.485130
C	-0.907132	5.827750	3.364551
C	-0.708618	5.478499	4.695185
C	0.581784	5.247685	5.174107
C	1.661693	5.375861	4.302869
C	1.476654	5.721441	2.963891
H	-1.916934	5.989077	2.996370
H	-1.564167	5.378945	5.354364
H	0.740757	4.967901	6.209587
H	2.669862	5.192066	4.658157
N	-0.157500	6.164132	-1.130582
N	-0.160200	6.166703	1.127029
H	-1.139452	5.978960	-0.970837
H	-1.145764	6.001016	0.967878
H	2.327715	5.797430	-2.295346
H	2.322870	5.802146	2.300104
C	0.595707	6.363076	-0.001448
S	2.243943	6.837879	0.000445

Table S3. Coordinates of (6,6)-CNT

C	4.95326	4.08576	0.72638
C	4.95269	4.08958	-0.70616
C	3.72593	3.88777	-1.38196
C	3.72703	3.15443	-2.62816
C	4.95172	2.67158	-3.14517
C	4.95206	1.42444	-3.85217
C	3.72668	0.73551	-4.01436
C	3.72719	-0.71044	-4.01516
C	4.95212	-1.40120	-3.86478
C	4.95155	-2.64891	-3.15874
C	3.72640	-3.14097	-2.64935
C	3.72645	-3.87559	-1.40391
C	4.95287	-4.08883	-0.73266
C	4.95312	-4.08586	0.69985
C	3.72756	-3.88473	1.37916
C	3.72899	-3.14621	2.62050
C	4.95378	-2.66209	3.13302
C	4.95276	-1.42220	3.84397
C	3.71325	-0.73747	4.03523
C	3.71356	0.71184	4.03502
C	4.95272	1.39872	3.85546
C	4.95363	2.63953	3.14640
C	3.72842	3.13245	2.64148
C	3.72816	3.87291	1.40119
C	2.48202	4.06199	0.71725
C	2.48200	4.05679	-0.68829
C	1.22858	3.89022	-1.39433
C	1.22900	3.16658	-2.61511
C	2.48146	2.63917	-3.11668
C	2.48156	1.41775	-3.81063
C	1.22904	0.72222	-4.02125
C	1.22905	-0.69644	-4.02015
C	2.48198	-1.39541	-3.82284
C	2.48091	-2.61716	-3.12949
C	1.22892	-3.15437	-2.63766
C	1.22856	-3.87644	-1.41593
C	2.48240	-4.05646	-0.71371
C	2.48140	-4.06258	0.69185
C	1.22897	-3.91433	1.40229
C	1.22755	-3.17917	2.63121
C	2.47645	-2.64299	3.13002
C	2.48272	-1.42602	3.82432
C	1.22241	-0.71903	4.02233
C	1.22240	0.69352	4.02187
C	2.48293	1.40351	3.83640
C	2.47587	2.62080	3.14282
C	1.22745	3.16731	2.65466
C	1.22905	3.89910	1.42376
C	-0.00000	4.11209	0.74054
C	-0.00000	4.09830	-0.70804
C	-1.22858	3.89023	-1.39433
C	-1.22900	3.16658	-2.61512
C	-0.00000	2.67582	-3.13770
C	-0.00000	1.41789	-3.85248
C	-1.22904	0.72222	-4.02126
C	-1.22905	-0.69645	-4.02016
C	-0.00000	-1.39647	-3.86513
C	-0.00000	-2.65391	-3.14948
C	-1.22892	-3.15437	-2.63766
C	-1.22856	-3.87645	-1.41592
C	-0.00000	-4.09905	-0.73289
C	-0.00000	-4.11217	0.71569
C	-1.22897	-3.91434	1.40229
C	-1.22755	-3.17917	2.63122
C	-0.00000	-2.67992	3.13043
C	-0.00000	-1.41132	3.85101
C	-1.22241	-0.71903	4.02233
C	-1.22240	0.69353	4.02187
C	-0.00000	1.39023	3.86386
C	-0.00000	2.65962	3.14403
C	-1.22745	3.16731	2.65467
C	-1.22905	3.89910	1.42376
C	-2.48202	4.06199	0.71725
C	-2.48199	4.05679	-0.68829
C	-3.72593	3.88777	-1.38196
C	-3.72703	3.15443	-2.62816
C	-2.48145	2.63917	-3.11668
C	-2.48155	1.41775	-3.81062
C	-3.72668	0.73551	-4.01436
C	-3.72719	-0.71044	-4.01516
C	-2.48198	-1.39541	-3.82283
C	-2.48090	-2.61716	-3.12949
C	-3.72640	-3.14097	-2.64934
C	-3.72645	-3.87559	-1.40391
C	-2.48240	-4.05646	-0.71370
C	-2.48140	-4.06257	0.69184
C	-3.72756	-3.88473	1.37916
C	-3.72899	-3.14621	2.62050
C	-2.47644	-2.64299	3.13002
C	-2.48272	-1.42603	3.82431
C	-3.71325	-0.73747	4.03522
C	-3.71356	0.71184	4.03502
C	-2.48293	1.40351	3.83639
C	-2.47587	2.62080	3.14282
C	-3.72842	3.13246	2.64148
C	-3.72816	3.87291	1.40119
C	-4.95326	4.08577	0.72639
C	-4.95269	4.08959	-0.70616
C	-6.16457	3.99114	-1.49125
C	-6.16260	3.30112	-2.66666
C	-4.95172	2.67158	-3.14517
C	-4.95206	1.42444	-3.85218
C	-6.16443	0.69595	-4.15703
C	-6.16289	-0.66736	-4.15807
C	-4.95212	-1.40119	-3.86479
C	-4.95155	-2.64891	-3.15874
C	-6.16405	-3.28568	-2.69102
C	-6.16312	-3.97736	-1.51656
C	-4.95287	-4.08884	-0.73267
C	-4.95312	-4.08587	0.69985
C	-6.16753	-3.98246	1.48041
C	-6.16637	-3.28880	2.65295
C	-4.95378	-2.66210	3.13302
C	-4.95276	-1.42220	3.84398
C	-6.16452	-0.69561	4.14937
C	-6.16280	0.66677	4.14989
C	-4.95272	1.39871	3.85546
C	-4.95363	2.63953	3.14640
C	-6.16778	3.27364	2.67700
C	-6.16606	3.96931	1.50564
H	-7.07410	4.43813	-1.09524
H	-7.07518	3.16866	-3.24766
H	-7.07575	1.26275	-4.33703
H	-7.07739	-1.23391	-4.33375
H	-7.07331	-3.15691	-3.27464
H	-7.07602	-4.42027	-1.11867
H	-7.07668	-4.42929	1.08334
H	-7.07934	-3.15218	3.23243
H	-7.07606	-1.26290	4.32786
H	-7.07767	1.23392	4.32341
H	-7.07747	3.14080	3.25901
H	-7.07836	4.41234	1.10680
C	6.16280	0.66677	4.14990
C	6.16453	-0.69560	4.14937
C	6.16637	-3.28880	2.65295
C	6.16753	-3.98246	1.48041
C	6.16312	-3.97736	-1.51656
C	6.16405	-3.28569	-2.69101
C	6.16289	-0.66736	-4.15808
C	6.16443	0.69595	-4.15704
C	6.16260	3.30113	-2.66666
C	6.16457	3.99114	-1.49125
C	6.16606	3.96931	1.50564
C	6.16778	3.27364	2.67700
H	7.07606	-1.26291	4.32788
H	7.07934	-3.15218	3.23244
H	7.07667	-4.42930	1.08334
H	7.07601	-4.42029	-1.11867
H	7.07331	-3.15692	-3.27466
H	7.07739	-1.23391	-4.33377
H	7.07575	1.26275	-4.33706
H	7.07518	3.16867	-3.24767
H	7.07410	4.43815	-1.09524
H	7.07836	4.41235	1.10680
H	7.07746	3.14081	3.25902
H	7.07767	1.23393	4.32343



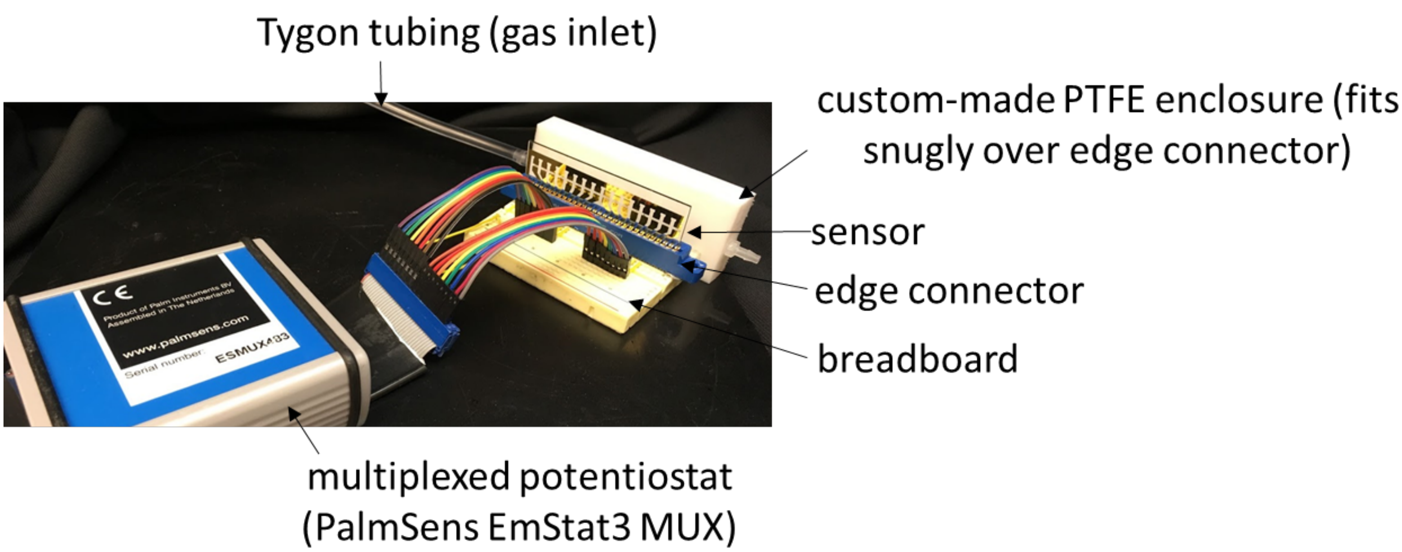


Figure S12. Sensor schematic (top) and device setup photo (bottom)

In the photo, the PTFE enclosure is placed to the side of the sensor for clarity. During operation, the enclosure fits snugly on the edge connector and directs the analyte stream to the sensor chip.

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