Supporting Information

Carboxylated Single-Walled Carbon Nanotube Sensors with Varying pH for the Detection of Ammonia and Carbon Dioxide using Artificial Neural Network

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Figure S1. Illustration of the PCB chip used with 16 wells for sensor material deposition. A diagram of the electrode shape is also included, showing an example of the bridge formed by the SWCNT-COOH network.

Figure S2. Schematic representation of the neural network model used to predict NH$_3$ and CO$_2$ concentrations from the sensor system. The model takes in two tensors, one 60 x 16 composed of raw data and the other 60 x 18 composed of processed data. The arrow points in the directions, which the tensors pass through the model. The inputs were passed first into separate GRU cells, which were then fed into the fully connected layers. The output is the prediction of the sensed CO$_2$ and NH$_3$ concentrations.
Figure S3. Normalized sensor response (R/R₀) to NH₃ and CO₂ exposures using H₃PO₄-pretreated SWCNT-COOH (pH 1.9 - blue) and NaOH-pretreated SWCNT-COOH (pH 9.1 - red). Exposed gas concentrations were 10, 30 and 75 ppm NH₃ and 1000, 3000 and 7500 ppm CO₂ at 24 °C. Relative gas concentrations are indicated by the bar heights. Relative humidity of (a) 22 %RH and (b) 0.7-9.4 %R
Calculation of the effect of dissolved CO$_2$ and NH$_3$ in solution

For calculating the effect of dissolved CO$_2$ on [H$^+$] in solution:

\[ CO_2(g) \rightleftharpoons CO_2(aq) \]

\[ H = \frac{[CO_2(aq)]}{P_{CO_2}} = 0.0344 \text{ mol} L \cdot \text{atm} \text{ or } k_H = \frac{P_{CO_2}}{[CO_2(aq)]} = 29.76 \text{ L} \cdot \text{atm} \text{ mol} \]

\[ CO_2(aq) + H_2O \rightleftharpoons H_2CO_3 \]

\[ K_H = \frac{[H_2CO_3]}{[CO_2(aq)]} \approx 1.7 \times 10^{-3} \]

\[ H_2CO_3 + H_2O \rightleftharpoons HCO_3^- + H^+ \]

\[ K_{a1} = 2.5 \times 10^{-4} \]

\[ HCO_3^- \rightleftharpoons CO_3^{2-} + H^+ \]

\[ K_{a2} = 4.69 \times 10^{-11} \]

\[ K_w = [H^+][OH^-] = 10^{-14} \]

According to the rule of charge neutrality and neglecting \([\text{CO}_3^{2-}]\):

\[ [H^+] = [OH^-] + [HCO_3^-] \]

\[ [H^+] = \frac{K_w}{[H^+] + K_{a1}[H_2CO_3]} \]

\[ [H^+]^2 = K_w + K_{a1}[H_2CO_3] \]

\[ [H^+]^2 = K_w + K_{a1}K_H[CO_2(aq)] \]

\[ [H^+]^2 = K_w + \frac{K_{a1}K_H}{K_H}P_{CO_2} \]

\[ [H^+] = \sqrt{10^{-14} + \frac{K_HK_{a1}}{K_H}P_{CO_2}} \]

For calculating the effect of dissolved ammonia on [H$^+$] in solution:

\[ NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^- \]

\[ K_b = 1.75 \times 10^{-5} \]

\[ \frac{[NH_4^+][OH^-]}{[NH_3]} = \frac{x^2}{[NH_3]-x} = K_b \]

\[ x = [OH^-] \]
\[ [H^+] = \frac{K_W}{[OH^-]} \]

**Figure S4.** Graphs showing calculated pH changes of water for given NH\textsubscript{3} concentration in ppm (blue line) and CO\textsubscript{2} concentration in ppm (red line).\textsuperscript{2} The respective changes in NH\textsubscript{4}\textsuperscript{+} concentration and H\textsubscript{2}CO\textsubscript{3} concentration are also shown (dashed lines). A higher target gas concentration results in a higher equilibrium concentration of [NH\textsubscript{4}\textsuperscript{+}] or [H\textsubscript{2}CO\textsubscript{3}]. Dotted lines show ppm values of target gases tested.

**Figure S5.** (a) UV-Vis absorption spectra of SWCNT and SWCNT-COOH solutions at various pH conditions. Spectra were normalized at 905 nm. Inset: Density of states diagram of metallic and semiconducting
SWCNTs demonstrating the transitional bands (M11, S11, and S22). (b) The S22 peak decreases at 975 nm as pH of the solutions increases. The S22 peak of pristine SWCNT/SDBS is higher than that of SWCNT-COOH at all pH conditions.

References
