Electronic Supplementary Information (ESI)

Evolution of ZnO microstructures from hexagonal disk to prismoid, prism and pyramid and their crystal facet-dependent gas sensing properties

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**Gas concentration calculation**

To obtain the desired gas concentration, injection volume of the gas or liquid can be calculated as follow:

When the test target is gas:

$$V_x = V \times C \times 10^{-6} \times \frac{273 + T_r}{273 + T_c}$$  \hspace{1cm} (1)

When the test target is liquid vapor:

$$V_x = \frac{V \times C \times M}{22.4 \times d \times p} \times 10^{-9} \times \frac{273 + T_r}{273 + T_c}$$  \hspace{1cm} (2)

where $V_x$ is the injection volume (ml), $V$ is the test chamber volume (ml), $C$ is the gas or liquid vapor concentration (ppm), $M$ is the liquid mole mass (g/mol), $d$ is the liquid specific gravity (g/cm$^3$), $p$ is the liquid purity, $T_r$ is the room temperature (°C) and $T_c$ is the chamber temperature (°C).
Gas sensing properties of the sensors

\[ \text{O}_2 \text{(gas)} \leftrightarrow \text{O}_2 \text{(adsorbed)} \]  
\[ \text{O}_2 \text{(ads)} + e^- \leftrightarrow \text{O}^- \text{(ads)} \]  
\[ \text{O}^- \text{(ads)} + e^- \leftrightarrow 2\text{O}^- \text{(ads)} \]  
\[ \text{O}^- \text{(ads)} + e^- \leftrightarrow \text{O}_2^- \text{(ads)} \]  
\[ \text{V}_\text{O} + \text{O}_2 \text{(g)} \leftrightarrow \text{O}_2^- \text{(ads)} + \text{V}_\text{O}^- \]  
\[ \text{V}_\text{O} + \text{O}_2 \text{(g)} \leftrightarrow \text{O}_2^- \text{(ads)} + \text{V}_\text{O}^- \leftrightarrow 2\text{O}^- + 2\text{V}_\text{O}^- \]

wherein “g” and “ads” refer to gas and adsorbate, \( \text{V}_\text{O} \) oxygen vacancy, and \( \text{V}_\text{O}^- \) single electropositive oxygen vacancy.

In addition, \( \text{C}_2\text{H}_5\text{OH} \) gas can be either dehydrated at the surface of acidic oxide:

\[ \text{C}_2\text{H}_5\text{OH} \text{(g)} \rightarrow \text{C}_2\text{H}_4 \text{(g)} + \text{H}_2\text{O} \text{(g)} \]  

or dehydrogenated at the surface of basic oxide:

\[ \text{C}_2\text{H}_5\text{OH} \text{(g)} \rightarrow \text{CH}_3\text{CHO} \text{(g)} + \text{H}_2 \text{(g)} \]  

Since ZnO is a basic metal oxide, the catalytic oxidation of \( \text{C}_2\text{H}_5\text{OH} \) on the ZnO surface will happen according to Eq. 10. The sequent gas sensing reaction is shown in Eq. 11:

\[ \text{CH}_3\text{CHO} \text{(ads)} + 5\text{O}^- \text{(ads)} \rightarrow 2\text{CO}_2 + 2\text{H}_2\text{O} + 5e^- \]  

When the sensor is exposed to the other gases:

\[ \text{H}_2 \text{(ads)} + \text{O}^- \text{(ads)} \rightarrow \text{H}_2\text{O} + e^- \]  
\[ \text{CH}_3\text{OH} \text{(ads)} + 3\text{O}^- \text{(ads)} \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} + 3e^- \]  
\[ \text{HCHO} \text{(ads)} + 2\text{O}^- \text{(ads)} \rightarrow \text{CO}_2 + \text{H}_2\text{O} + 2e^- \]