

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:

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

When the test target is liquid vapor:

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

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/cm³), 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



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

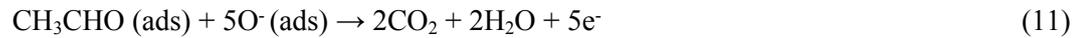
In addition, $\text{C}_2\text{H}_5\text{OH}$ gas can be either dehydrated at the surface of acidic oxide:



or dehydrogenated at the surface of basic oxide:



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:



When the sensor is exposed to the other gases:

