Role of the heterojunctions in In$_2$O$_3$-composited SnO$_2$ nanorod sensors and their remarkable gas-sensing performance for NO$_x$ at room temperature

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The $I_{ds}$-$V_{ds}$ measurements device equipped with two removable probes placed directly on the electrode contact areas on the substrate, as shown in Figure S1. The interdigital Au electrode spacing is 2 µm.

![Figure S1 Device structure of $I_{ds}$-$V_{ds}$ measurement](image1)

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![Figure S2 The diagram of the gas delivery system for the gas sensing process](image2)

Figure S2 The diagram of the gas delivery system for the gas sensing process
Figure S3 SEM image of (A) 1ICTO and (B) 5ICTO.

Figure S4 TEM image of 3ICTO. The arrows point out pores. The SnO$_2$ nanoparticles (NPs) dispersed on the surface of 3ICTO. The sizes of SnO$_2$ NPs is about 5-20 nm (see the diameter distribution of 3ICTO in Figure S6B).

Figure S5 HRTEM images of (A) 1ICTO and (B) 5ICTO in which (110), (200) and (101) planes of SnO$_2$, (222) and (400) planes of In$_2$O$_3$ can be seen.
Figure S6 (A) element maps of the 3ICTO NRs (B) the nanoparticles diameter distribution of 3ICTO NRs, the inset of (B) shows the SAED pattern of SnO$_2$ NPs.

Figure S7 The XPS full spectra (A) and O1s spectra of (B): (a) pristine SnO$_2$, (b) 1ICTO, (c) 3ICTO, (d) 5ICTO.

Table S1. XPS results of pristine In$_2$O$_3$ and various ICTOs.

<table>
<thead>
<tr>
<th>samples</th>
<th>In$<em>{3d</em>{5/2}}$ (eV)</th>
<th>In$<em>{3d</em>{3/2}}$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In$_2$O$_3$</td>
<td>443.8</td>
<td>451.4</td>
</tr>
<tr>
<td>1ICTO</td>
<td>444.6</td>
<td>452.2</td>
</tr>
<tr>
<td>3ICTO</td>
<td>444.8</td>
<td>452.4</td>
</tr>
<tr>
<td>5ICTO</td>
<td>444.8</td>
<td>452.4</td>
</tr>
</tbody>
</table>

Figure S8 (A) UV–vis diffuse reflection–absorption curves; (B) plot of $(\alpha h\nu)^2$ versus incident photon energy $(h\nu)$ for the ICTOs (the pristine SnO$_2$ (black line) and 1ICTO (red line), 3ICTO (blue line), and 5ICTO (green line)).
The band gap energy of a semiconductor could be calculated by equation (eq) 1

\[ a \, h \nu = K (h \nu - E_g)^n \]  
\[ (1) \]

Where \( E_g \) is the band gap energy, \( h \nu \) is the incident photon energy, \( K \) is a constant, \( \alpha \) is the absorption coefficient. In the eq.1, \( n \) decides the characteristics of the transition in a semiconductor. In the case of SnO\(_2\), the value of \( n \) is 1 due to a direct optical transition type for SnO\(_2\). Therefore, by plotting \((a\nu)^2\) versus \(h\nu\), the band gap \((E_g)\) can be determined (as shown in Figure S8B).

The carrier concentration also can be calculated by the slope of the MS curves using the following eq2.

\[ N_a = \left( \frac{2}{\varepsilon e \varepsilon_0} \right) \left( \frac{1}{d(V/C^2)/dV} \right) \]  
\[ (2) \]

where \( e_0 \) is the fundamental charge constant, \( \varepsilon_0 \) is the permittivity of vacuum, \( \varepsilon \) is the relative permittivity of SnO\(_2\) (\( \varepsilon = 23.4 \)).

Table S2 Carrier concentrations and fitted impedance parameters of the SnO\(_2\), 1ICTO, 3ICTO and 5ICTO

<table>
<thead>
<tr>
<th>Samples</th>
<th>( R_0 (\Omega) )</th>
<th>( R_{ct} (\Omega) )</th>
<th>( N_a (\text{cm}^{-3}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>SnO(_2)</td>
<td>540.8</td>
<td>6130</td>
<td>( 3.25 \times 10^{19} )</td>
</tr>
<tr>
<td>1ICTO</td>
<td>403.3</td>
<td>3186</td>
<td>( 3.79 \times 10^{19} )</td>
</tr>
<tr>
<td>3ICTO</td>
<td>263.8</td>
<td>116.6</td>
<td>( 9.32 \times 10^{19} )</td>
</tr>
<tr>
<td>5ICTO</td>
<td>334.5</td>
<td>138.6</td>
<td>( 4.46 \times 10^{19} )</td>
</tr>
</tbody>
</table>

Figure S9 I-V curves measured at RT for (a) 3ICTO and (b) pristine SnO\(_2\) thin film sensors, which were treated at 60 °C, 250 °C and 400 °C in Ar.

Figure S9 shows the current-voltage (I\(_{ds}\)-V\(_{ds}\)) characteristics for a 3ICTO and pristine SnO\(_2\) were measured by sweeping the drain voltage from -10 V to 10 V with constant \( V_g = 1.0 \) V in 0.05 V steps.
Figure S10 Dynamic response-recovery curves of the pristine SnO$_2$ sensor to 100 ppm-3 ppm NO$_x$ at RT

Figure S11 Work functions of the (A) pristine SnO$_2$ and (B) pristine In$_2$O$_3$

References