Electronic Supplementary Information (ESI) for RSC Advances.

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Butane detection: W-doped TiO_2 nanoparticles for butane gas sensor with high sensitivity and fast response/recovery

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Table S1. Structural data and refinement parameters for 5%W-TiO_2 nanoparticles calculated by Rietveld refinement of the experimental XRD powder pattern.

Space group	$I4_1/amd$ (141)
Lattice parameters	
a (Å)	3.7928
b (Å)	3.7928
c (Å)	9.5064
Ti/W	
x	0
y	0
z	0
O	
x	0
y	0
z	0.2126
Average crystallite size (nm)	7.75
Average maximum strain (10^{-3})	3.735
R_{WP} (%)	19.6
R_P (%)	14.4

Table S2. The fitted equation for different sensors.

Sample	m	k	R^2
TiO_2	-0.0066	5.6816	0.9639
2.5%W-TiO_2	-0.0063	5.5390	0.9835
5.0%W-TiO_2	-0.0097	6.3100	0.9950
7.5%W-TiO_2	-0.0067	5.1750	0.9793

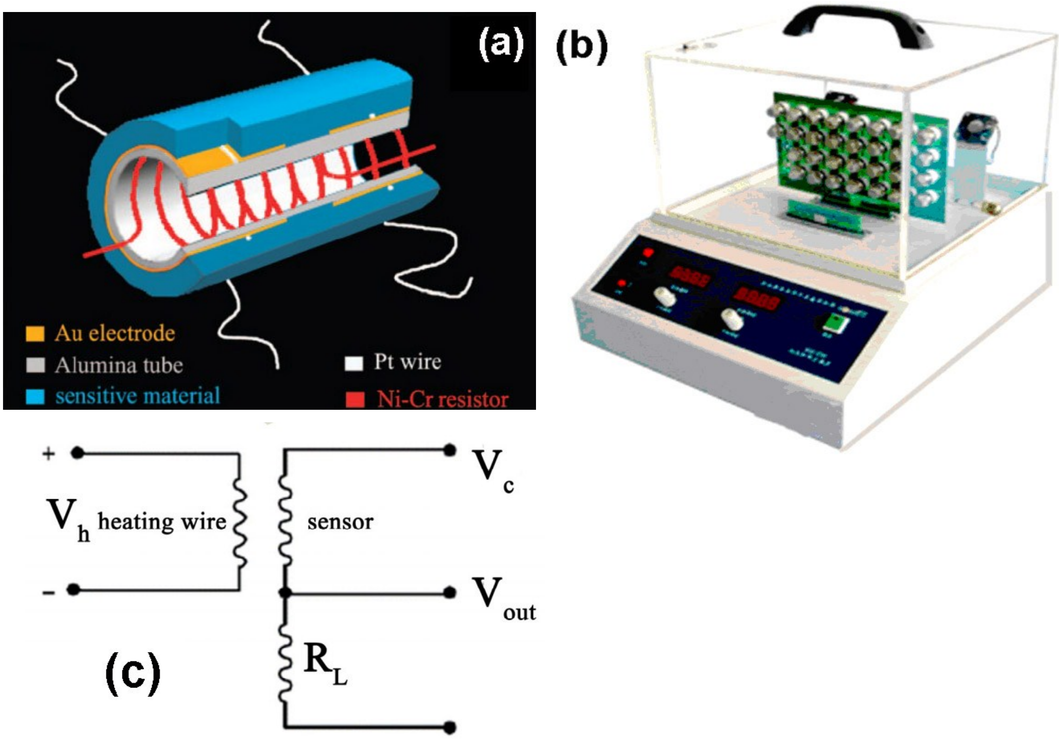

Fig. S1 (a) the schematic structure of the gas sensor, (b) A photograph of the WS-30 A testing system, (c) the basic testing principle (where V_h is the heating voltage, R_L is a constant load resistance, V_{out} is the sensor export voltage, and V_c is the working voltage (5V).)

According to Fig. S1(c), the electrical resistance of the sensor can be calculated as following:

$$R = \frac{5 - V_{\text{out}}}{V_{\text{out}}} \cdot R_{\text{L}}$$

And the gas response defined as the ratio of the resistance of the sensor in air (R_0) to that in gas (R_g):

$$R_0 = \frac{5 - (V_{\text{out}})_{\text{air}}}{(V_{\text{out}})_{\text{air}}} \cdot R_{\text{L}}\,, \quad R_{\text{g}} = \frac{5 - (V_{\text{out}})_{\text{g}}}{(V_{\text{out}})_{\text{g}}} \cdot R_{\text{L}}\,, \quad \beta = \frac{R_0}{R_{\text{g}}}$$

where $(V_{out})_{air}$ is the export voltage in air, and $(V_{out})_{gas}$ is that in gas.

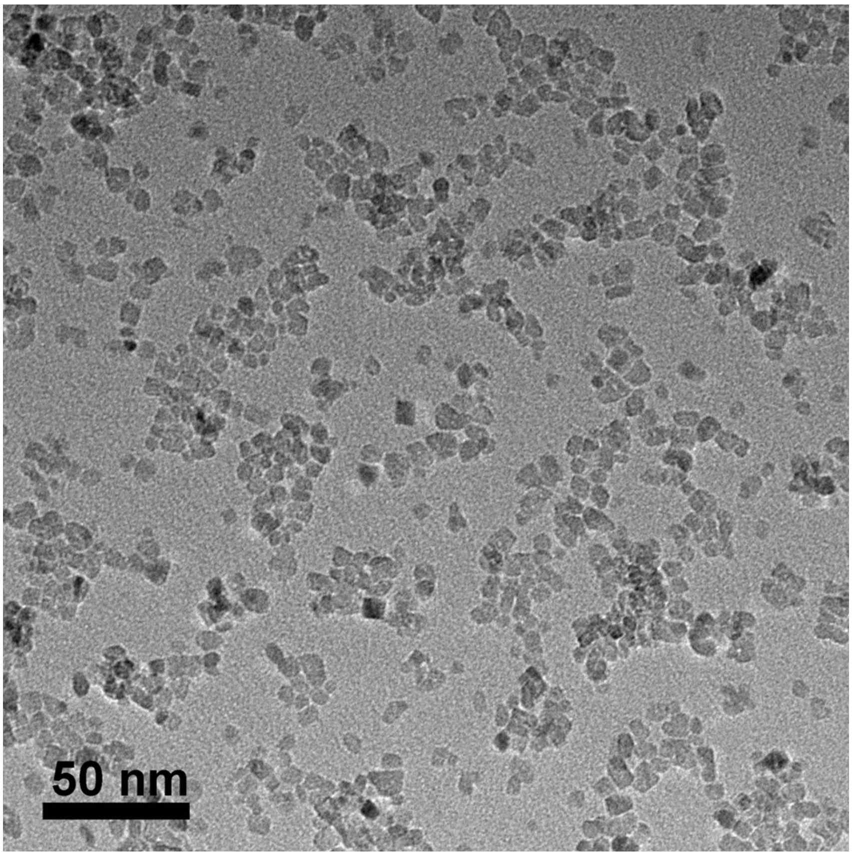

Fig. S2 TEM imagine of as-prepared pure TiO_2 nanoparticles.

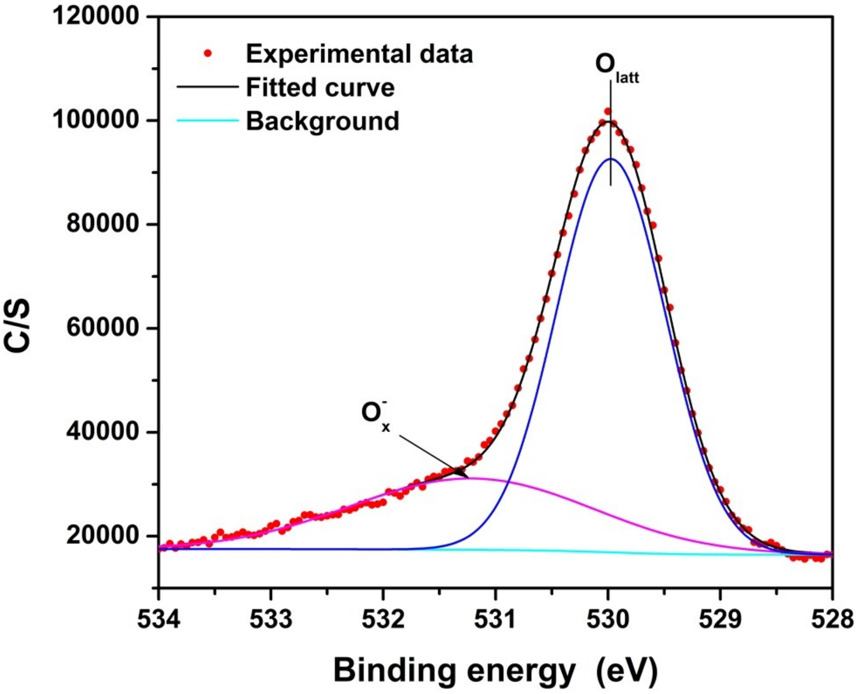

Fig. S3 High-resolution XPS spectra of O1s of as-prepared pure TiO_2 nanoparticles.

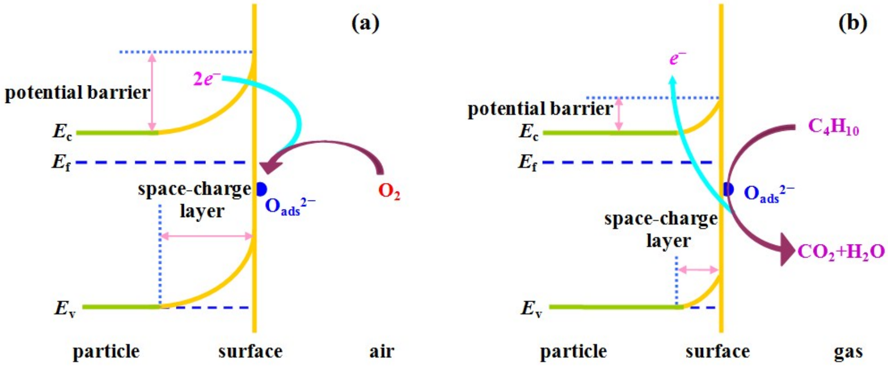

Fig. S4 Schematic diagram of the butane sensing mechanism.

The oxygen species absorbed from air onto the surface of TiO_2 nanoparticle capture the free electrons from the sensing materials, which leads to the formation of absorbed oxygen ions (O_x^-, O_{ads}^- or O_{ads}^{2-}) and a consequent thick space layer as well as a high resistance of the sensor. During these processes, following reactions happens:

$$O_{2gas} \leftrightarrow O_{2ads}$$

$$O_{2ads} + e^- \leftrightarrow O_{2ads}^-$$

$$O_{2ads}^- + e^- \leftrightarrow 2O_{ads}^-$$

$$O_{ads}^- + e^- \leftrightarrow O_{ads}^{2-}$$

When the sensor exposed to butane, butane would react with the formed absorbed oxygen ions and the captured electrons would be released, leading to a thinner space-charge layer. Such the process results in a decrease of the resistance and can be described as following equations:

$$(C_4H_{10})_{gas} \leftrightarrow (C_4H_{10})_{ads}$$

$$(C_4H_{10})_{ads} + 13O_{ads}^- \rightarrow 4CO_2 + 5H_2O + 13e^-$$

$$(C_4H_{10})_{ads} + 13O_{ads}^{2-} \rightarrow 4CO_2 + 5H_2O + 26e^-$$