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Supplementary Materials

Influence of Nickel Doping on Ultrahigh Toluene Sensing Performance of Core-Shell ZnO Microsphere Gas Sensor

Zhenhua Li [1], Sijia Li [1], Zijian Song [1], Xueli Yang [1,*], Ziyan Wang [1], Hao Zhang [2], Lanlan Guo [3], Caixuan Sun [1], Hongyan Liu [1], Junkai Shao [1], Yehong Cheng [4,*] and Guofeng Pan [1]

[1] Tianjin Key Laboratory of Electronic Materials and Devices, School of Electronics and Information Engineering, Hebei University of Technology, 5340 Xiping Road, Beichen District, Tianjin 300401, China
[2] Tianjin Key Laboratory of Materials Laminating Fabrication and Interface Control Technology, School of Materials Science and Engineering, Hebei University of Technology, Tianjin 300130, China
[3] School of Physics and Electronic Information Engineering, Henan Polytechnic University, Jiaozuo 454003, China
[4] School of Mechanical Engineering, Hebei University of Technology, Tianjin 300401, China
* Correspondence: xlyang@hebut.edu.cn (X.Y.); chengyehong@hebut.edu.cn (Y.C.)

All liquid samples in this experiment were analytical reagents. To obtain a 100 ppm VOC gas sample, the required volume of liquid can be calculated by Equation (1). The calculation results are shown in Table S1.

$$C_{ppm} = \frac{22.4 \times \varphi \times \rho \times V_1}{M \times V_2} \times 1000 \quad (1)$$

where C_{ppm} is the concentration of the desired gas; φ is the mass fraction of the analytically pure liquid corresponding to the gas; ρ and M are defined as the density and molecular weight of the analytically pure liquid, respectively; V_1 (μL) represents the volume of the analyte liquid to be added to the test chamber; V_2 is the volume of the test chamber (V_2 = 1 L). After the required liquid volume is obtained by calculation, analytically pure liquids are injected into the glass chamber through a micro syringe, and the liquid is volatilized to form a gas. Subsequently, the sensing performance test is carried out.

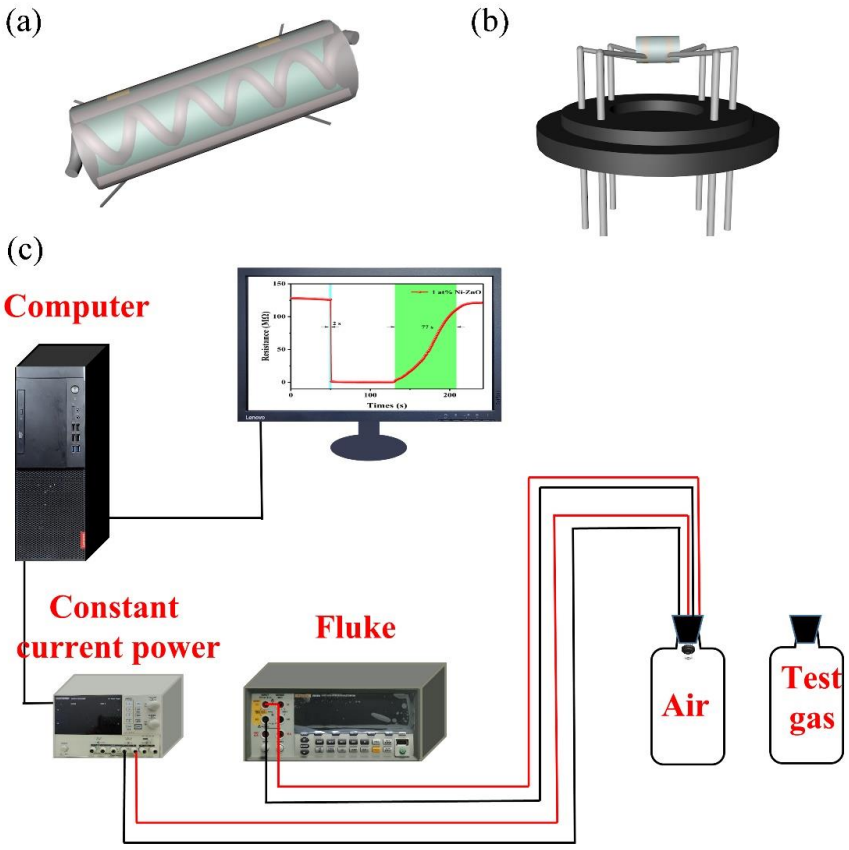

Figure S1. The schematic figure of the (**a**) ceramic tube, (**b**) sensor device, and (**c**) the sensing test system.

The diffuse reflectance spectrum in the wavelength range of 200~800 nm was studied by UV–Vis spectrophotometry. Figure S2a is the UV–Vis absorbance spectra of the four materials, where compared with the pure ZnO, the absorption peak of 600–700 nm existed in the samples, corresponding to Ni–ZnO. The band gap of the samples was calculated according to the Kubelka–Munk formula in Figure S2b. The band gap of the 0, 0.5, 1, and 2 at% Ni–ZnO was calculated to be 3.05, 2.98, 2.89, and 2.94 eV, respectively. The band gap of ZnO decreased with Ni doping. With the reduction in the band gap, the energy needed for free electrons released from the conduction band becomes less, and the electronic transition becomes easier. The electrical conductivity of the material increases, which might lead to generating a higher sensing response.

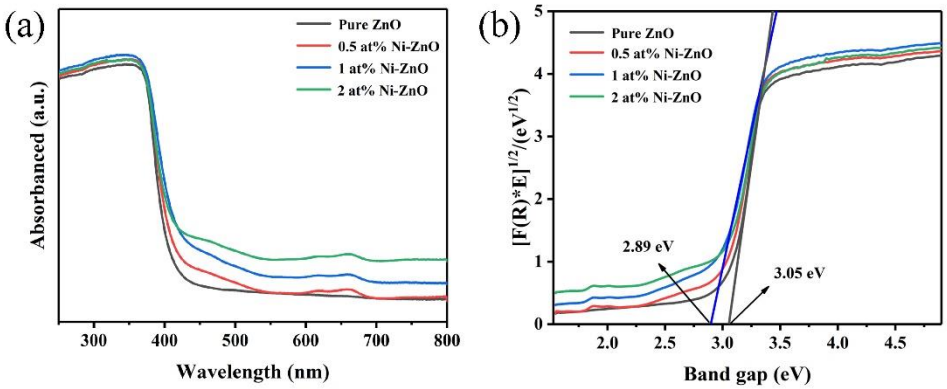

Figure S2. (**a**) The UV–Vis absorption spectrum and (**b**) energy band gap of the ZnO samples with different Ni doping amounts.

Table S1. The parameter information for all of the gas samples.

Gas	C (ppm)	φ (%)	M (g mol^{-1})	ρ (g cm^{-3})	V_1 (μL)
Toluene	100	≥99.5	92.14	0.866	0.477
Ethanol	100	≥99.7	46.07	0.789	0.261
Acetone	100	≥99.5	58.08	0.788	0.330
Methanol	100	≥99.5	32.04	0.792	0.181
Formaldehyde	100	37.0	30.03	1.083	0.334
Xylene	100	≥99.0	106.17	0.860	0.556