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The modification effect of Fe_2O_3 nanoparticles on ZnO nanorods improves the adsorption and detection capabilities of TEA

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The details of theoretical simulation

Our calculations performed in this paper were within the first-principles plane-wave pseudopotential density functional theory (DFT) as implemented in the VASP code. The projected augmented wave (PAW) method was employed and the generalized gradient approximation (GGA) Perdew-Burke-Ernzerhof (PBE) was used to describe the exchange-correlation interactions. A plane-wave cut-off energy (500 eV) for the expansion of the wave function into plane waves and a proper Monkhorst-Pack k-meshes sampled in the Brillouin zone were used to ensure the maximum atomic force in the system is less than 0.01 eV/atom and the energy difference of two iterations is less than 10^{-4} eV/atom.

The gas sensing testing process

1. Preparation of the testing gases

The desired concentrations of the testing gases (**acetone, methanal, ammonia, benzene, ethanol and methanol**) were obtained by the static gas distribution method, which was calculated by the following formula :

$$Q = \frac{V \times \varphi \times M}{22.4 \times \mathrm{d} \times \rho} \times 10^{-9} \times \frac{273 + T_R}{273 + T_B} \qquad (1)$$

where Q (mL) is the liquid volume of the volatile compound or gas volume, V (mL) is the volume of the testing chamber, φ is the required gas volume fraction, M (g mol^{-1}) is the molecular molar mass, d ($g \cdot cm^{-3}$) is the specific gravity, and ρ is the purity of the volatile testing liquid or gas, T_R and T_B (℃) are the temperatures at ambient and the test chamber, respectively.

2. Measurement of gas sensing

When the resistance of the sensor became stable, a certain amount of test gases were injected into the test bottle using a syringe. After waiting for 20 minutes, put the gas sensor into the test bottle to measure corresponding resistance. The sensor then was took out and exposed to clean air in a testing chamber without analytes, which in a ventilated indoor environment.

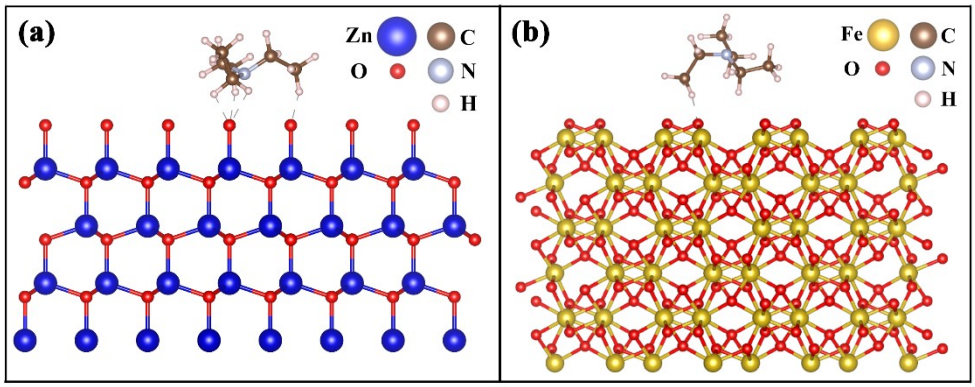

Fig. S1 The adsorption models to TEA molecule: (a) pure ZnO and (b) pure Fe_2O_3.

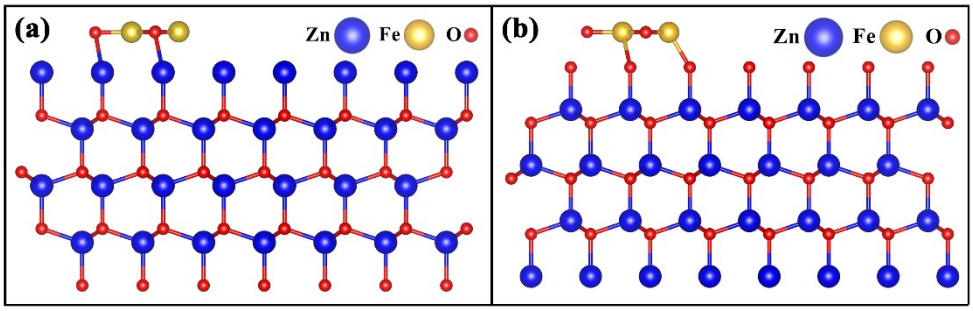

Fig. S2 The structural models of (a) M_{Zn} and (b) Mo.

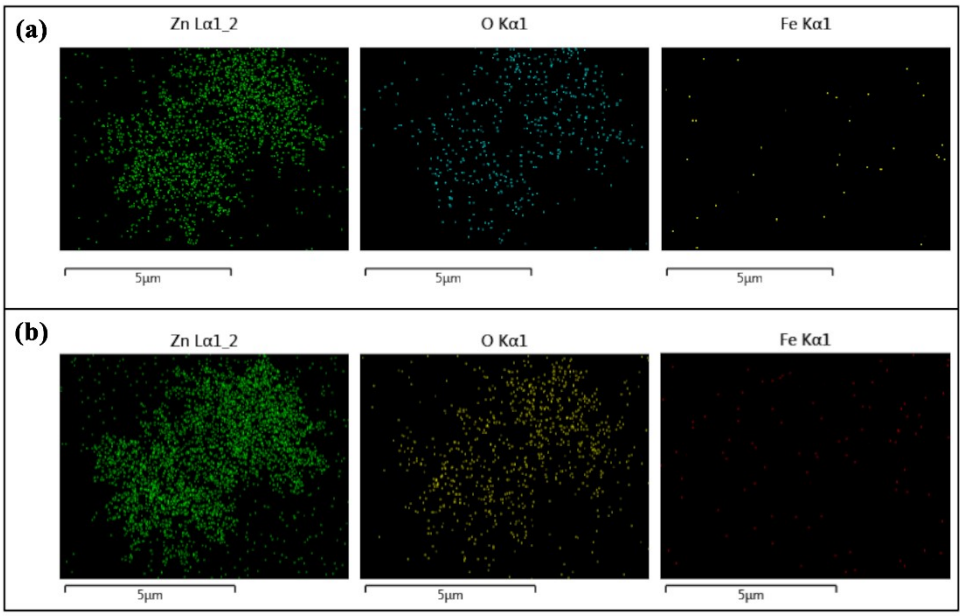

Fig. S3 The EDS image of (a) 1 wt% Fe_2O_3/ZnO and (b) 4 wt% Fe_2O_3/ZnO.

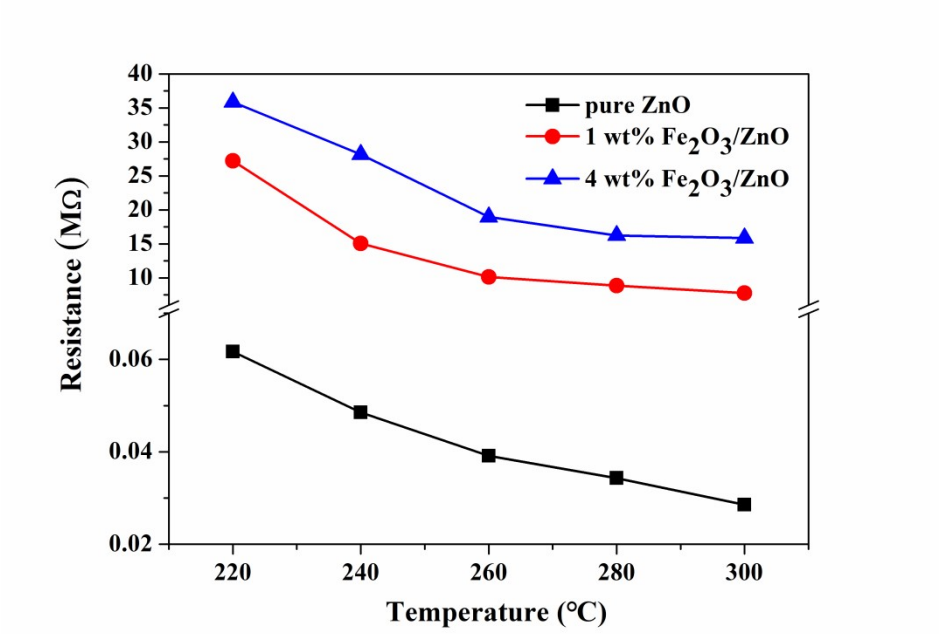

Fig. S4 The transient resistance of the pure ZnO, 1 wt% Fe_2O_3/ZnO and 4 wt% Fe_2O_3/ZnO in the air at different operating temperatures.

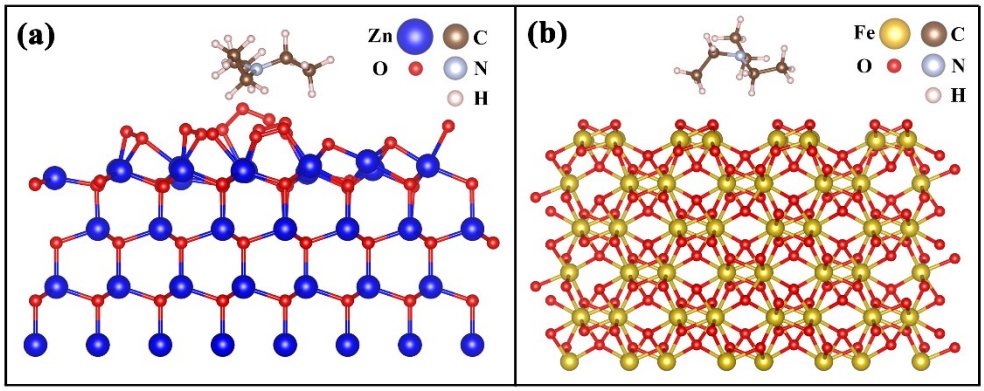

Fig. S5 The optimized adsorption models to TEA: (a) pure ZnO and (b) pure Fe_2O_3.

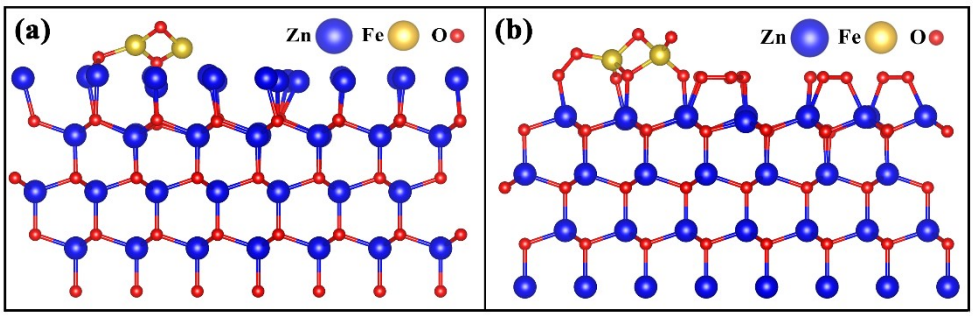

Fig. S6 The optimized structural models of (a) M_{Zn} and (b) Mo.

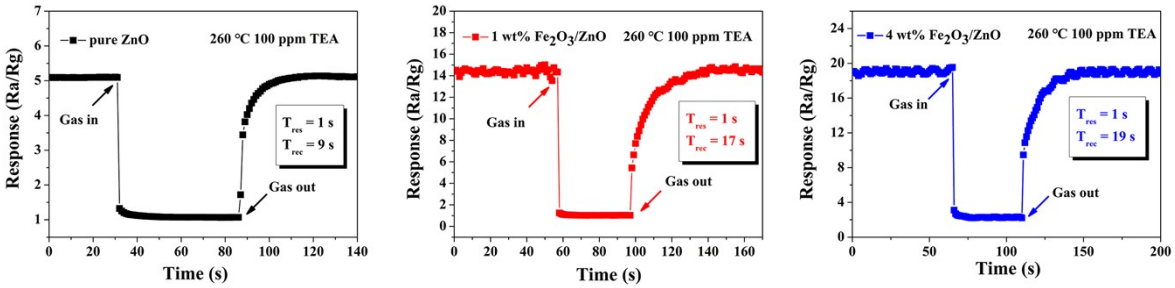

Fig. S7 The response curves of the sensors after 35 days.