Supplementary Materials

Topological insulator modified nickel oxide nanoflowers for low-temperature hydrogen sulfide gas sensing

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First-principles calculation methods

In this work, we utilized first-principles calculations based on density functional theory (DFT) to elucidate the gas sensitivity of NiO_x and Bi_2Te_3@NiO_x. The CASTEP software package was employed to determine the adsorption energy and charge density differences of these materials. The Perdew-Burke-Ernzerhof (PBE) functional, coupled with D2 dispersion correction, was selected to account for exchange-correlation effects. Ultrasoft pseudopotentials were utilized to model electron-ion interactions, while a plane-wave basis set was applied for the expansion of the Kohn-Sham orbitals. The Monkhorst-Pack K-point grid was sampled at densities of $2\pi\times0.04$ Å^{-1} and $2\pi\times0.02$ Å^{-1} for geometry optimizations and electronic structure calculations, respectively. A kinetic energy cut-off of 400 eV was established for these calculations. The structural optimization was considered complete when the total energy convergence reached 10^{-5}eV, and the force on each atom was below 0.01 eV Å^{-1}. To avoid interactions between adjacent periodic images, a 20 Å vacuum space was incorporated into the model. Furthermore, the band structure was computed using the VASP software, with the inclusion of spin-orbit coupling (SOC) to provide a comprehensive analysis.

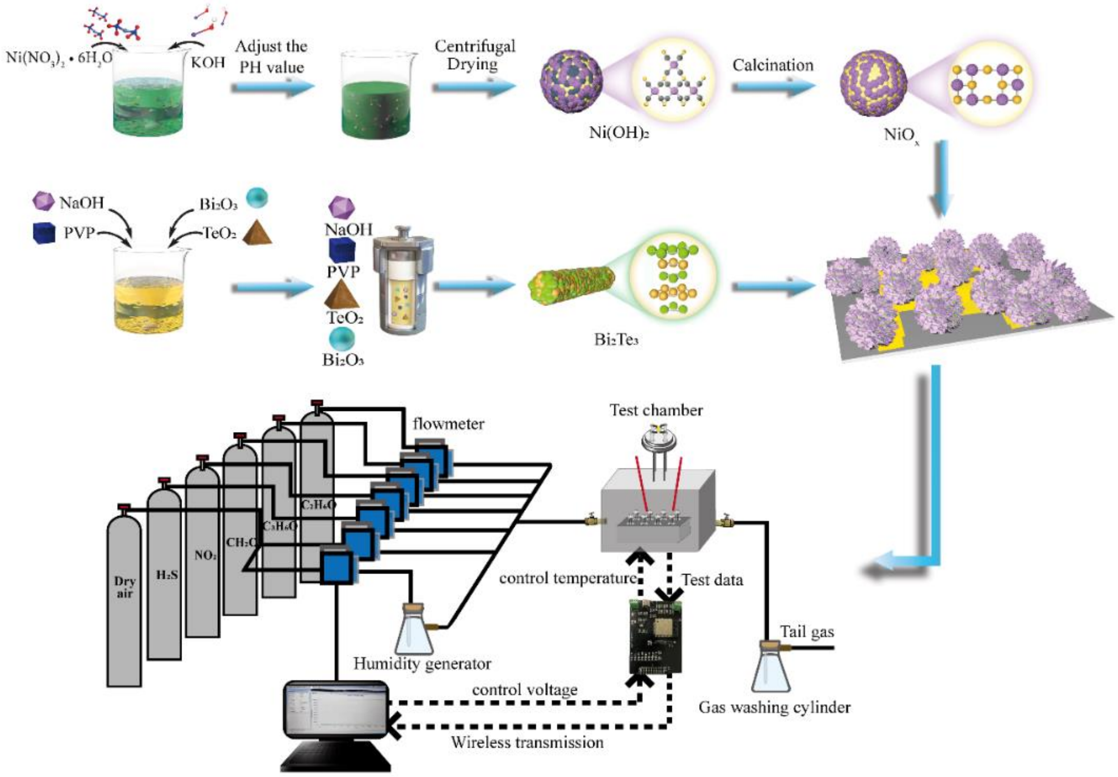

Figure S1. Schematic diagram of the synthesis of Bi_2Te_3@NiO_x and the testing system.

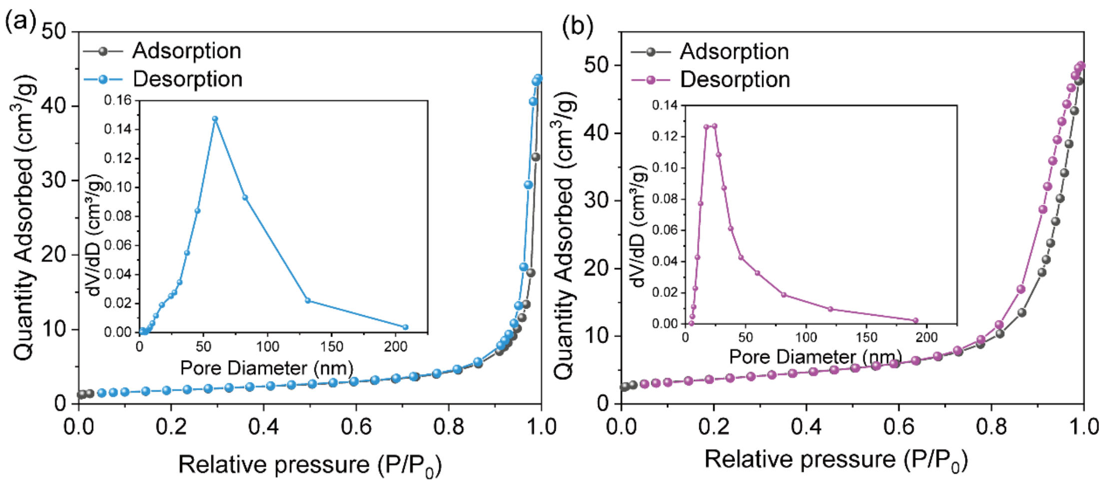

Figure S2. N_2 adsorption–desorption isotherms and pore size distribution curves of pure NiO_x (a) and 10 wt% Bi_2Te_3@NiO_x (b).

Table S1. The comparison among our work and recent H_2S gas sensors

Materials	T (°C)	Resp.	Con. (ppm)	LOD (ppm)	Ref.
SnO_2	160	5	9	3	[1]
NiO	175	5.8	100	3	[2]
Nb_2O_5@ZnO	400	6.1	20	1	[3]
WO_3	300	1.84	100	-	[4]
CuO-WO_3	300	6.72	100	-	[4]
rGO/CuO	300	11.7	10	1	[5]
SnO_2/RGO: Pt	200	3.7	40	1	[6]
Bi_2Te_3@NiO	90	11.81	10	0.2	This work

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