Supplymentary Material

Engineering Band Structure of SnO_2 Nanoparticles via Coupling with g-C_3N_4 Nanosheet for the Detection of Ethanolamine

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Computational Details

The band structure and density of states of the heterojunction formed by SnO_2 and g-C_3N_4 were analyzed theoretically. The Vienna Abinitio Simulation Package (VASP) and the super soft pseudopotential of the projection enhanced wave (PAW) are used to carry out density functional theory (DFT) calculation, and Perdew-Burke-Ernzerhof (PBE) is used as generalized gradient approximation (GGA) for commutative associated potential energy.[33] Other information can be referred to details (Supporting Information).

The Monkhorst Pack k-mesh of 4×4×4 for g-C_3N_4 (001) surfaces and 12×12×5 for SnO_2 (001) surfaces was used. The cut-off energy of the plane wave base is set to 400eV, and the total energy converges to 10^{-5} eV. When the residual force is less than 0.01 eV $Å^{-1}$, all atoms relax completely. The effective energy band structure and density of states (DOS) of g-C_3N_4, SnO_2 and g-C_3N_4/SnO_2 materials were obtain by processing the energy band calculation results based on the VASPKIT code.[34]

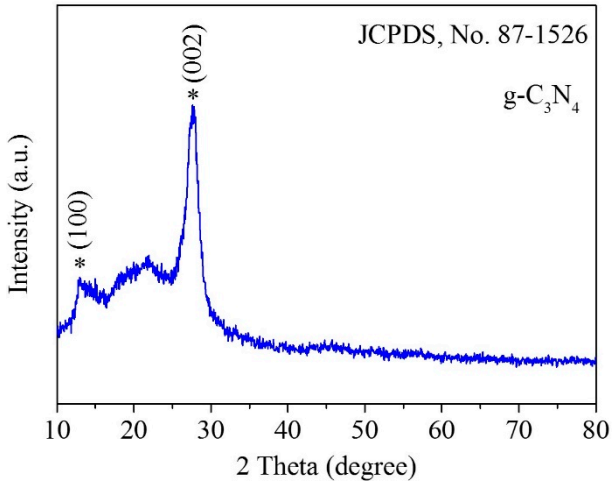

Figure S1 XRD patterns of g-C_3N_4

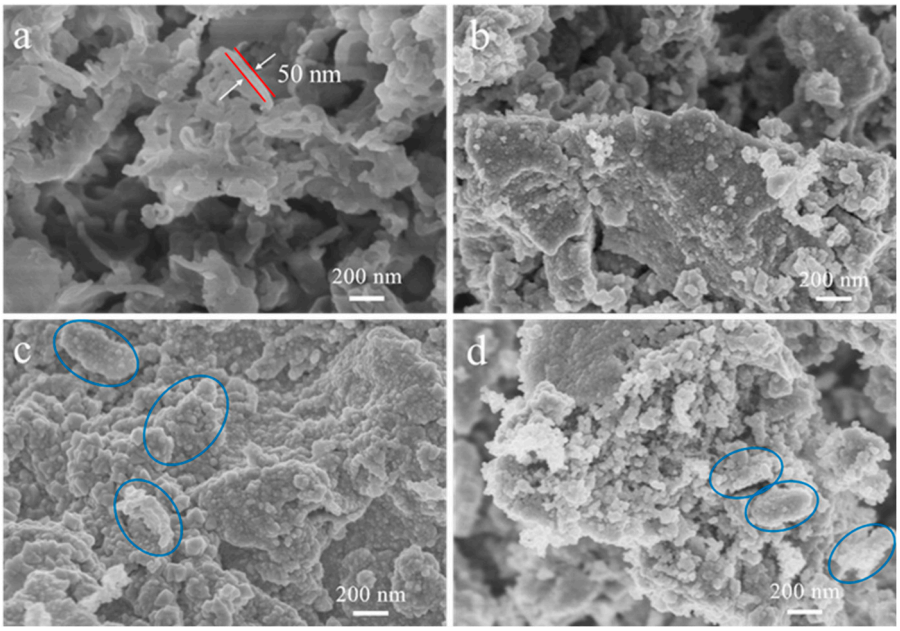

Figure S2 SEM images of as-synthesized materials (a) g-C_3N_4,(b) SnO_2, (c) g-C_3N_4/SnO_2-2.5 and (d) g-C_3N_4/SnO_2-10

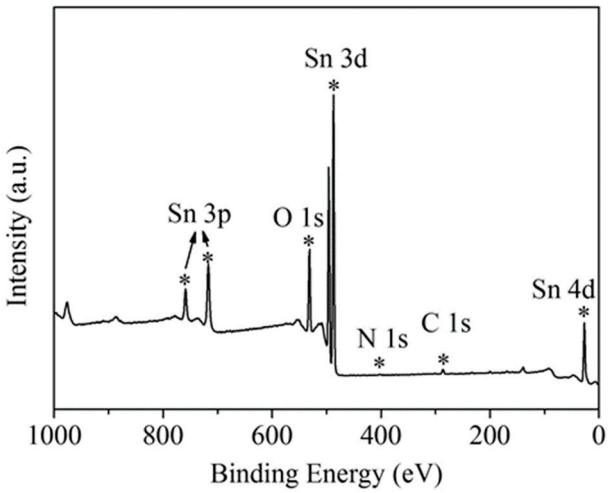

Figure S3 XPS spectra of the full range spectrum of g-C_3N_4/SnO_2-5 material

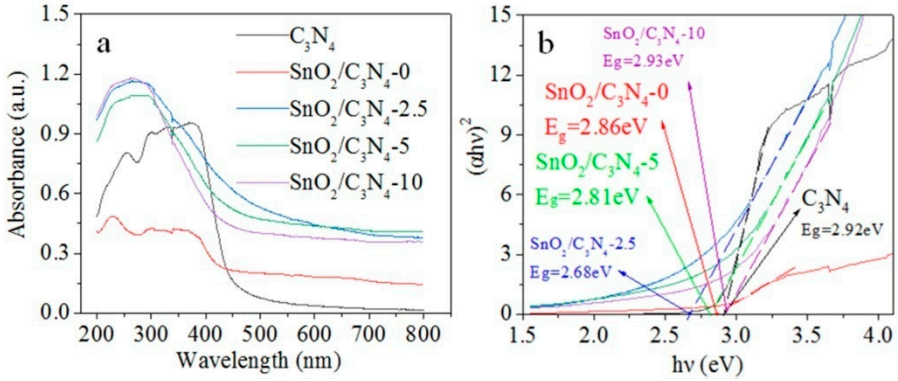

Figure S4 (a) UV–Vis absorption spectra of g-C_3N_4, SnO_2 and g-C_3N_4/SnO_2 and (b) bandgap energy of g-C_3N_4, SnO_2 and g-C_3N_4/SnO_2

References

[33] Liangruksa, M.; Sukpoonprom, P.; Junkaew, A.; Photaram, W.; Siriwong, C. Gas sensing properties of palladium-modified zinc oxide nanofilms: A DFT study, Appl. Surf. Sci. 2021,544,148868. https://doi.org/10.1016/j.apsusc.2020.148868.

[34] Wang, V.; Xu, N.; Liu, J. C. VASPKIT: A user-friendly interface facilitating high-throughput computing and analysis using VASP code, Computer Phys. Commun., 2021,267, 108033.