Supporting Information

Tailoring Pt-Loaded MoS$_2$/SnO$_2$ Heterostructures for High-Sensitivity Room-Temperature Ammonia Detection: A DFT and COMSOL Analysis

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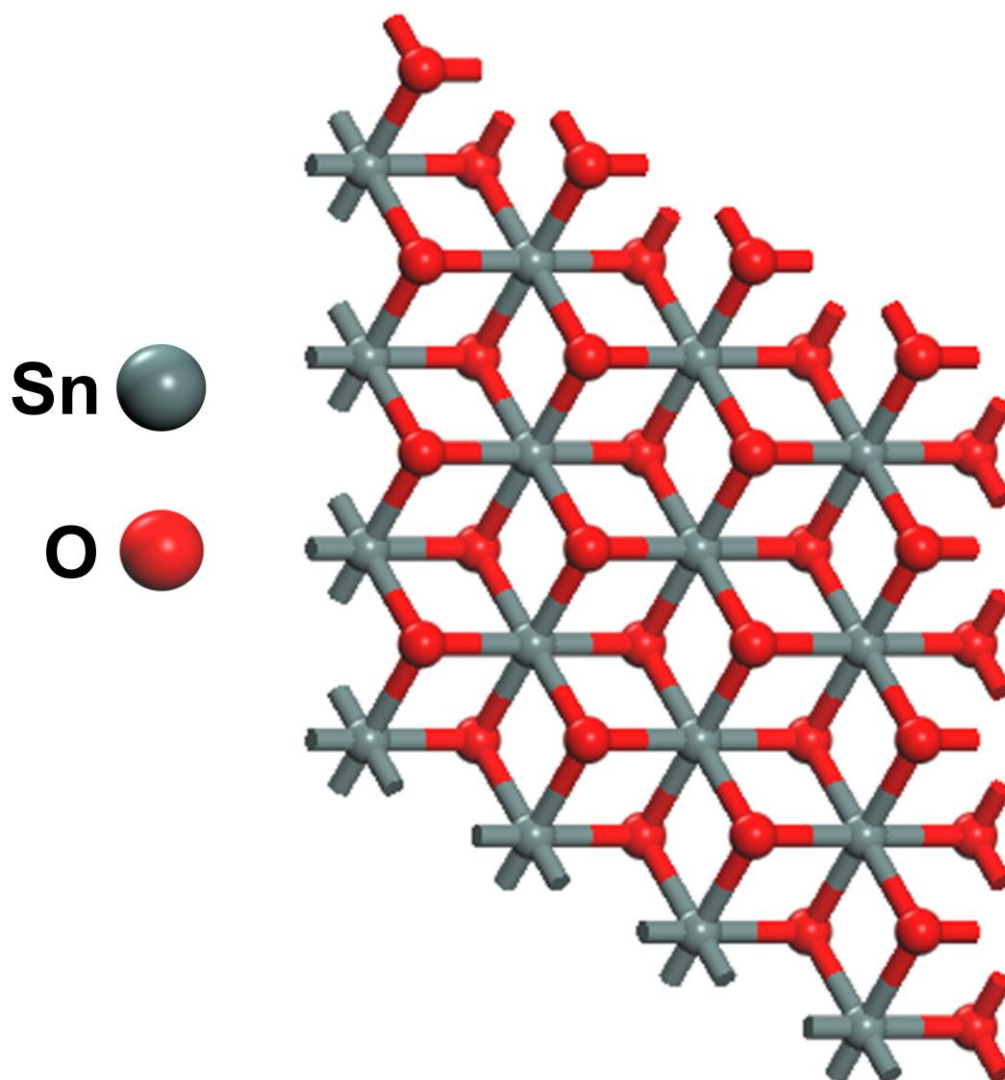*Corresponding Author: tawabur@eee.kuet.ac.bd

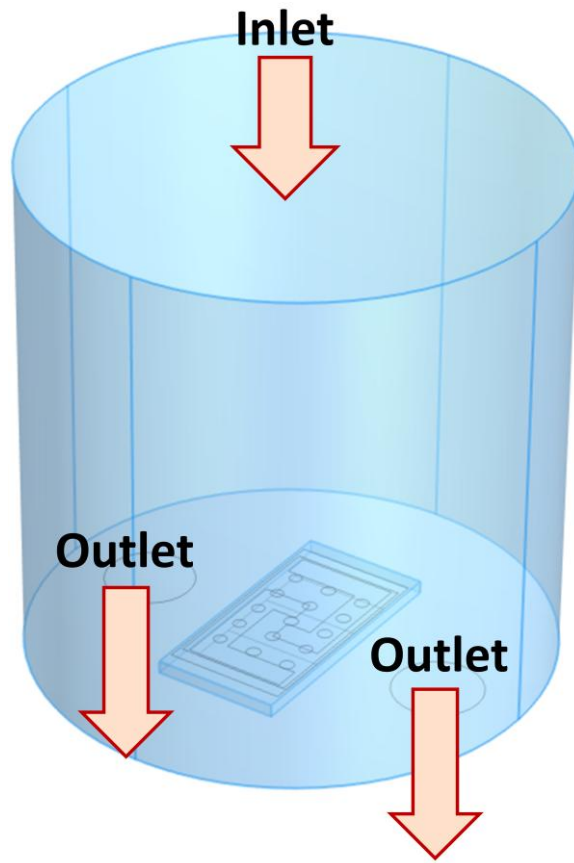Fig. SI1. 2D hexagonal SnO$_2$ monolayer (top view).

Fig. SI2. Gas chamber model of the proposed gas sensor.

Table S I The lattice constant; bond lengths of Mo-S (d_1) and Sn-O (d_2); bond angles of Mo-S-Mo (θ_1), S-Mo-S (θ_2), Sn-O-Sn (θ_3), and O-Sn-O (θ_4); the band gap (E_g); and VBM/CBM positions.

Lattice Constant (Å)	d_1(Å) d_2(Å)	θ_1(°) θ_2(°) θ_3(°) θ_4(°)	Interlayer Distance (Å)	E_g (eV)	Stability	VBM/CBM Positions
a = b = 6.24	2.401 2.008	80.82° 83.16° 101.57° 78.45°	3.36	2.063	Dynamically Stable	M/Γ
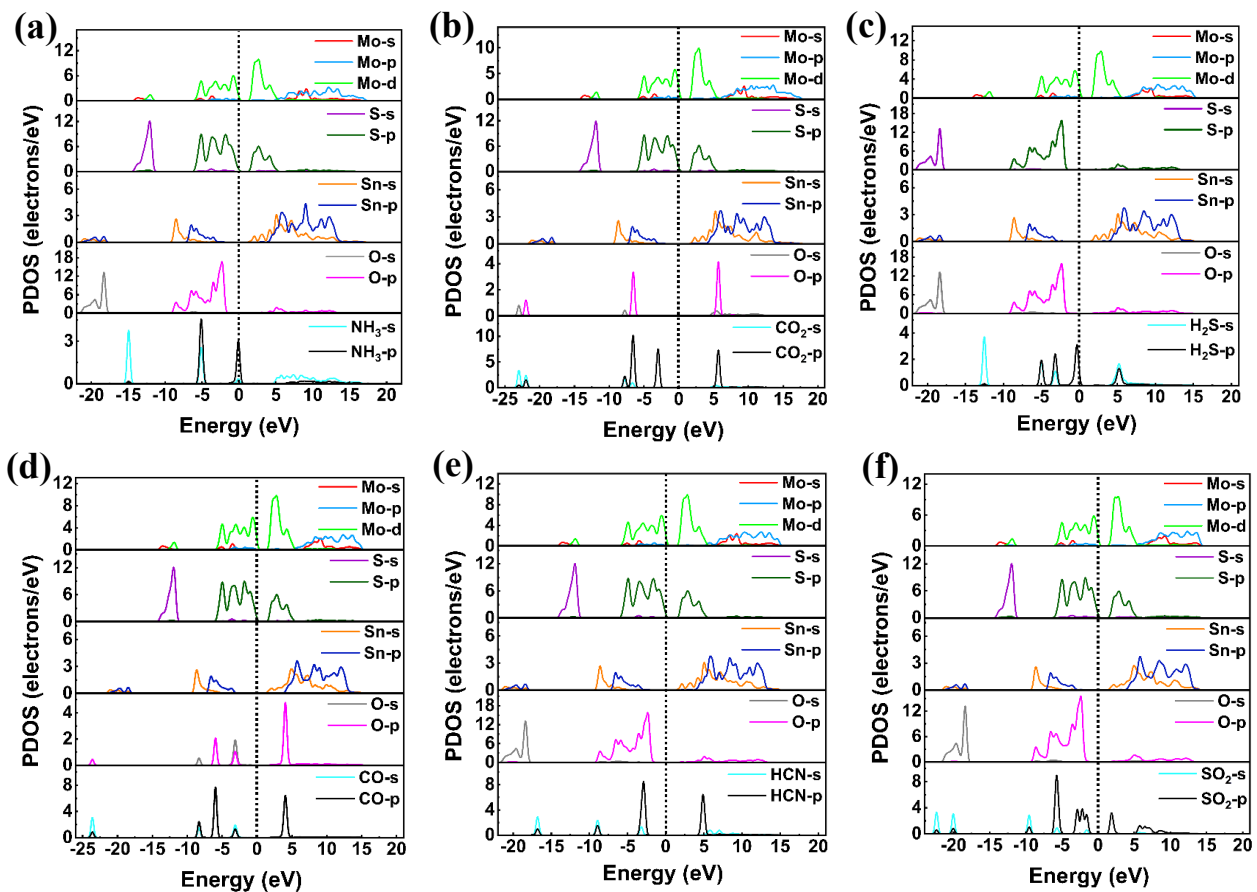
Fig. SI3. The PDOS of MoS$_2$/SnO$_2$ heterostructures adsorbed with (a) NH$_3$, (b) CO$_2$, (c) H$_2$S, (d) CO, (e) HCN, and (f) SO$_2$ molecules.
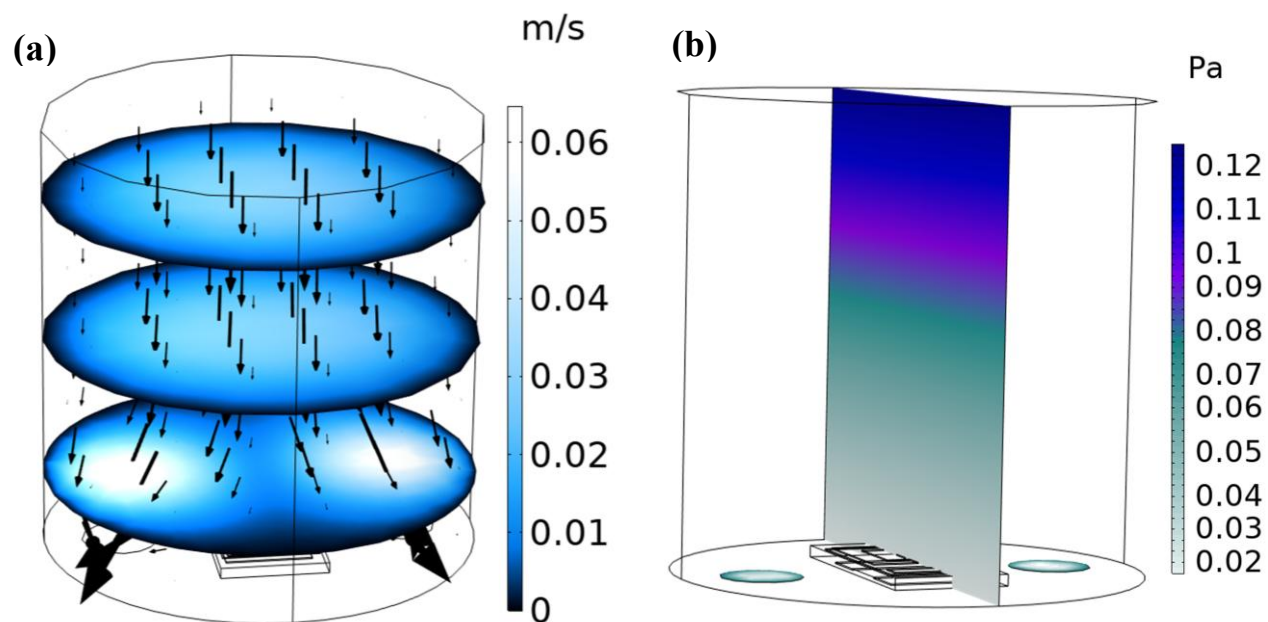
Fig. SI4 (a) Velocity and (b) pressure distribution of NH_3 gas as it flows through the gas chamber from the inlet to the outlet
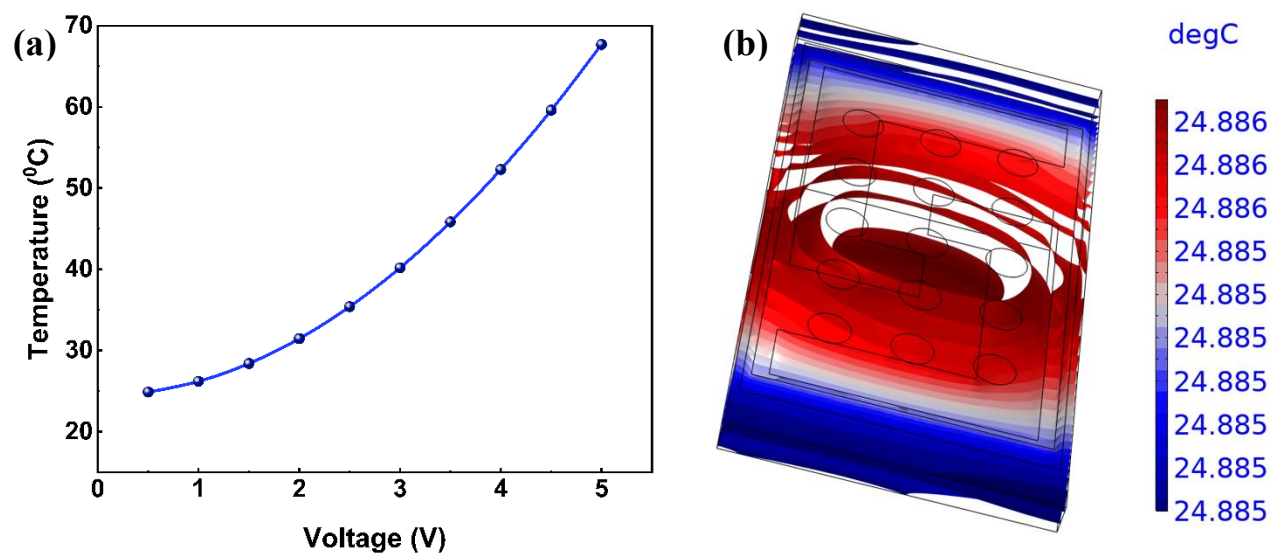

Fig. SI5. (a) Temperature versus voltage characteristics of the Pt-MoS$_2$/SnO$_2$ sensor for varying heater voltage from 0.5 to 5 V. (b) Isothermal contour of the sensor surface at 0.5 V.