Supporting Information

Tunable Gas Sensing Features of Janus In_2STe Monolayers: Insights from First-Principles and Multiphysics Studies on SO_2 Interaction

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Table SI The lattice constant; bond lengths of In-S (d_1), In-In (d_2), and In-Te (d_3); bond angles of In-S-In (θ_1), In-Te-In (θ_2), S-In-In (θ_3), and Te-In-In (θ_4); the band gap (E_g); VBM/CBM positions; and stability.

Lattice Constant (Å)	**d_1 (Å)** **d_2 (Å)** **d_3 (Å)**	**θ_1(°) θ_2(°)** **θ_3(°) θ_4(°)**	**Thickness, t (Å)**	**E_g (eV)**	**VBM/CBM Positions**	**Stability**
a = b = 4.16	2.53 2.73 2.75	103.36° 92.19° 115.02° 123.72°	5.37	1.402	Γ/Γ	Dynamically Stable

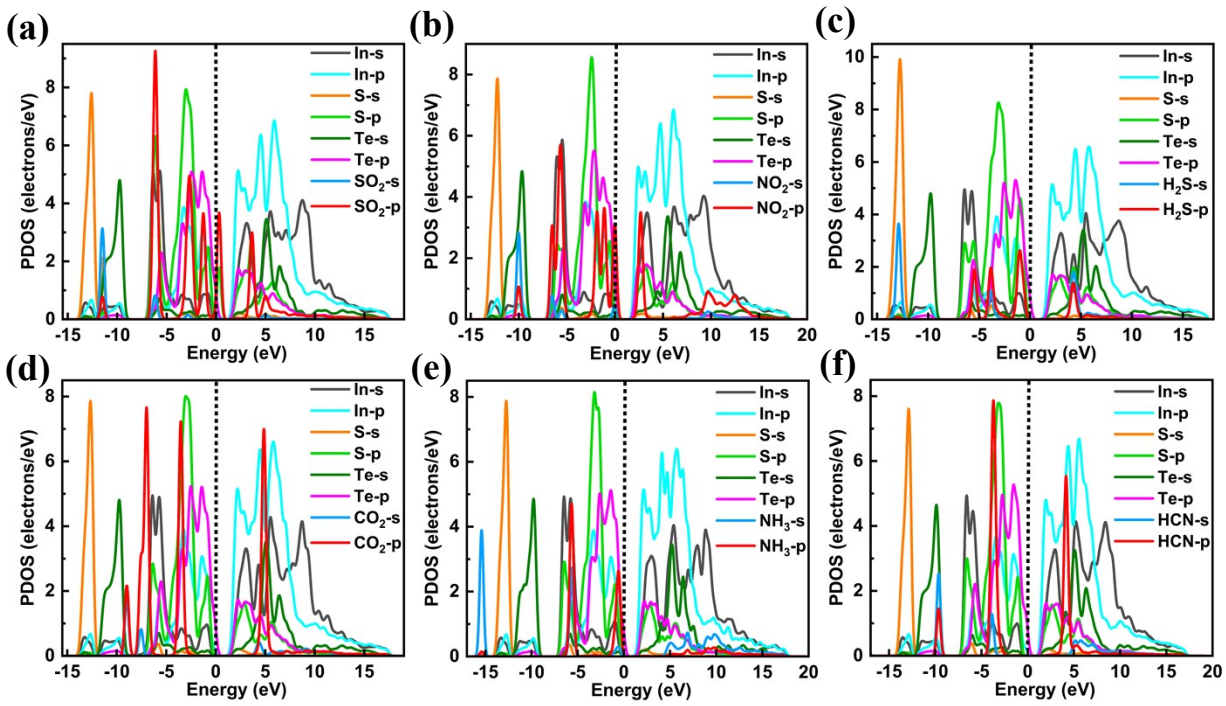

Fig. SI1. The PDOS of Janus In_2STe adsorbed with (a) SO_2, (b) NO_2, (c) H_2S, (d) CO_2, (e) NH_3, and (f) HCN molecules.

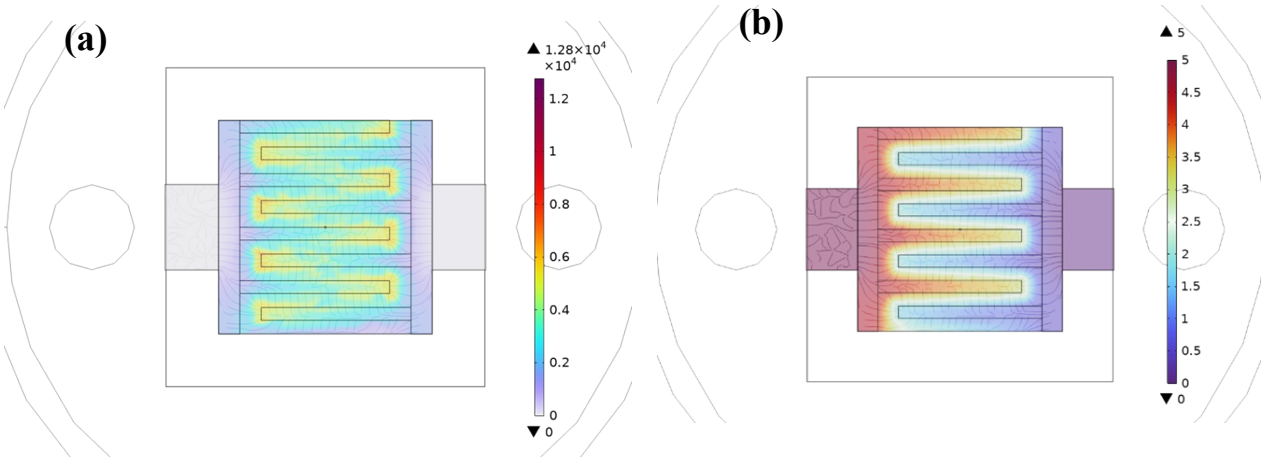

Fig. SI2. (a) Electric field distribution in the interdigitated Sensor (b) Electric potential distribution in the interdigitated Sensor.