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SUPPLEMENTRAY INFORMATION

Tellurene based Chemical Sensor

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Materials Characterization. A metallurgical microscope (CEWEI) was used to obtain optical images of samples. TEM were performed using JEM2100F operated at 200 kV. The incident energy of the electron beam was between 1 and 10 kV. AFM (Bruker, Innova) was used to characterize the morphology and measure the thickness of the samples. Raman spectroscopy was taken in a back-scattering geometry using a single monochromator with a microscope (Reinishaw inVia) equipped with CCD array detector (1,024 × 256 pixels, cooled to -70ºC) and an edge filter. The samples were excited by 514 nm Argon ion laser. X-ray diffraction patterns were obtained from a Bruker D2 PHASER using Cu/K α radiation (λ = 1.5418 Å) at 40 kV and 30 mA.

Materials Transfer and Device Fabrication. The substrates are fabricated using highly n-type-doped silicon wafers with ~300 nm thermally oxidized layer. The metal electrodes are deposited on the substrates by projection lithography and the minimum gap width is about 1 μm. Two pads (2 mm × 2 mm) are designed for connecting with external probes. Tellurene flakes were transferred to Polydimethylsiloxane (PDMS) by dropwise deposition method. Then a specific tellurene flake on PDMS was chosen under an optical microscope. The chosen tellurene was transferred to the 1 μm channel by alignment transfer method[23]. In the dry transfer process, only PDMS was used which did not contaminate the materials. The substrate with a heating electrode is shown in **Figure S2**. The current flowing through the heating resistor is ~50 mA when the heater is working, and the resistance of the heating resistor is ~50 Ω under cool condition.

Theoretical Calculations. The crystal structure of phosphorene (BP) and MoS_2 was obtained from crystallography open database.[1] The crystal structure of tellurene was obtained from previous work.[2] All of the theoretical calculations were performed by the QuantumATK package. The linear combination of atomic orbitals (LCAO) basis set is PseudoDojo pseudopotential combined with the generalized gradient approximation (GGA) with the

parametrization of Perdew-BurkeErnzerhof (PBE).[3,4] The Van der Waals correction is Grimme DFT-D2.[5] The mesh cut-off energy is 125 Ha and k-point grid is 3 × 3 × 1 for the relaxation calculation. We used the Limited-memory Broyden Fletcher Goldfarb Shanno (LBFGS) algorithm with the maximum stress tolerance value of 0.02 eV/Å^3. The electric current through the contact region is calculated using the Landauer-Buttiker formula implemented in the QuantumATK package.[6]

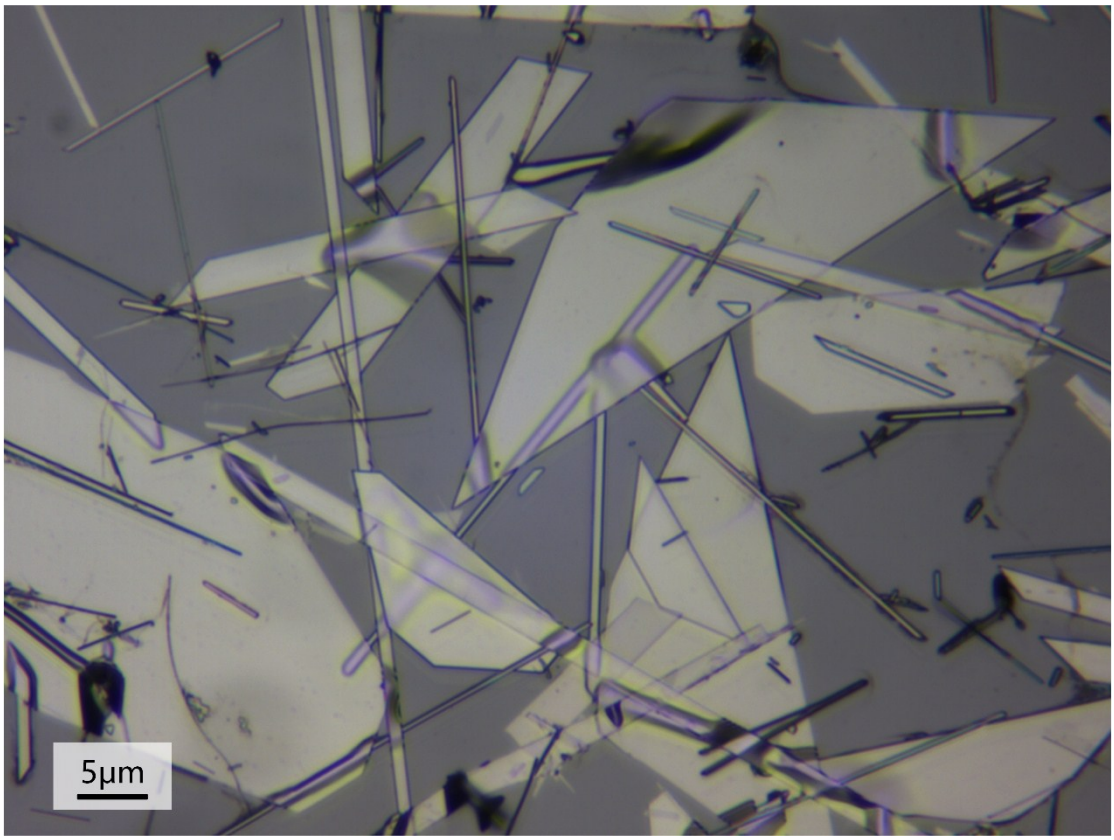

Figure S1. Typical optical image of tellurene sheets prepared by hydrothermal synthesis.

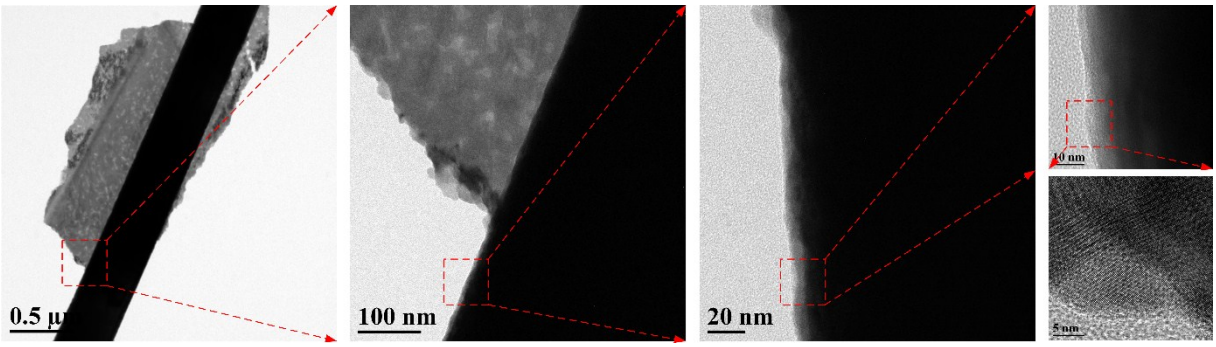

Figure S2. Different scales TEM images of tellurene flakes.

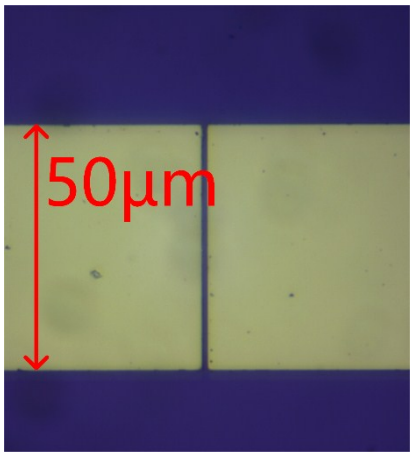

Figure S3. Optical image of the micro-nano electrode with a 1 μm gap.

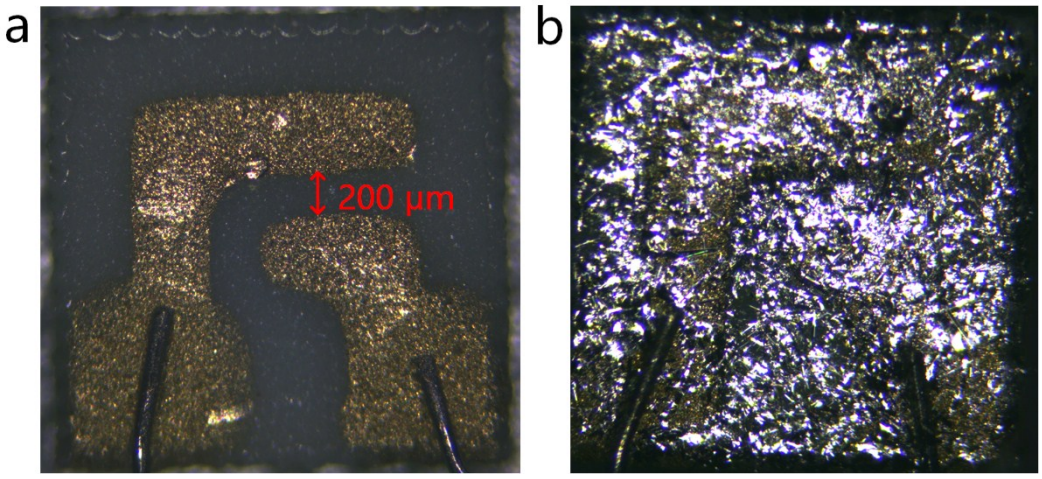

Figure S4. Optical image of substrate with a heating electrode on the back: **a**. clean substrate and **b**. the substrate with tellurene (the sliver grey powder) on the surface.

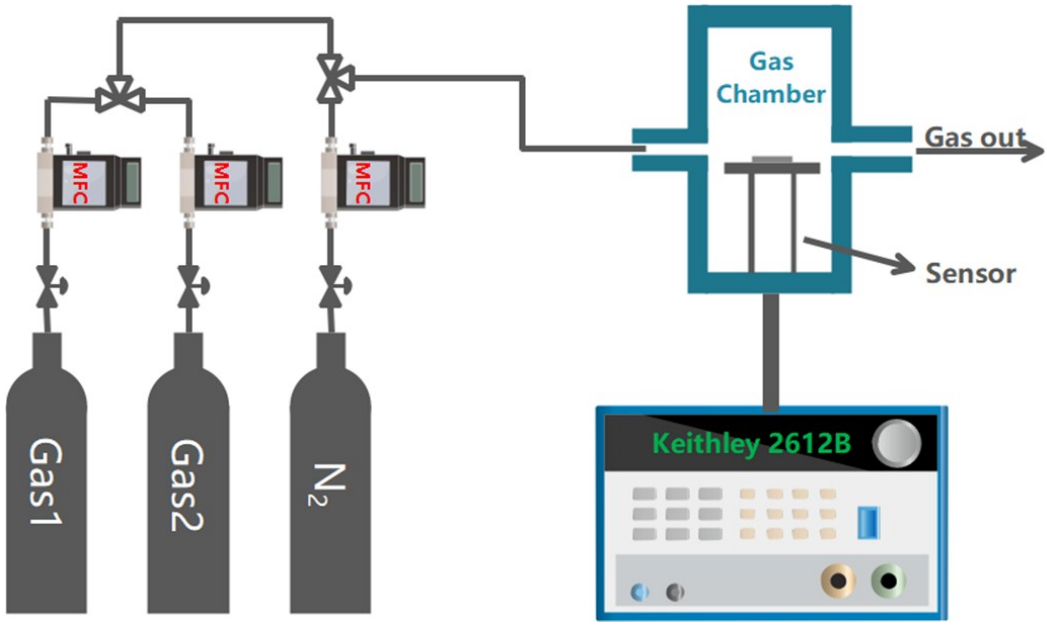

Figure S5. Schematic diagram illustrating the gas sensing test platform.

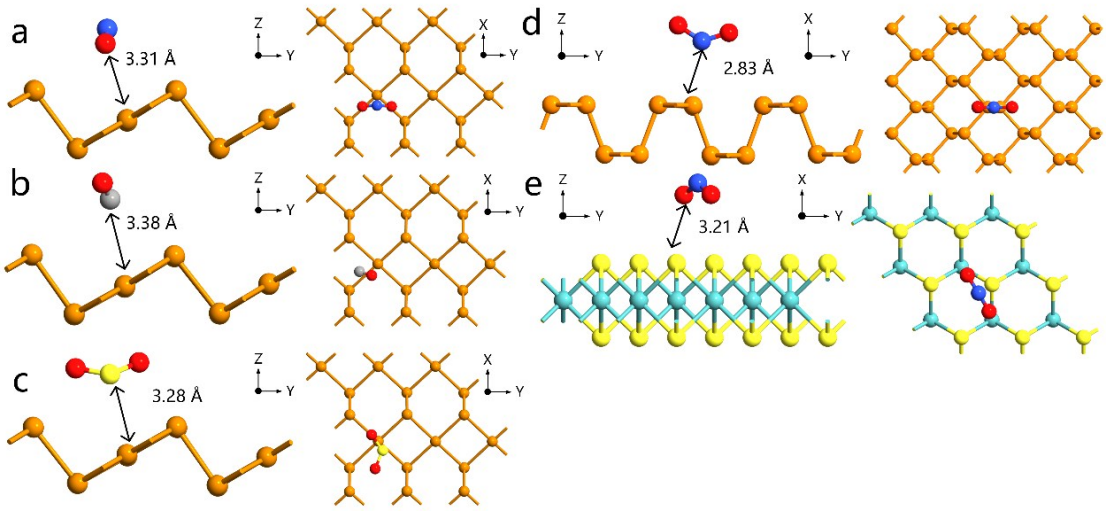

Figure S6. The optimized adsorption structures (front view and top view) of different adsorption systems: **a**. NO_2 adsorption on tellurene. **b**. CO adsorption on tellurene. **c**. SO_2 adsorption on tellurene. **d**. NO_2 adsorption on phosphorene. **e**. NO_2 adsorption on MoS_2.

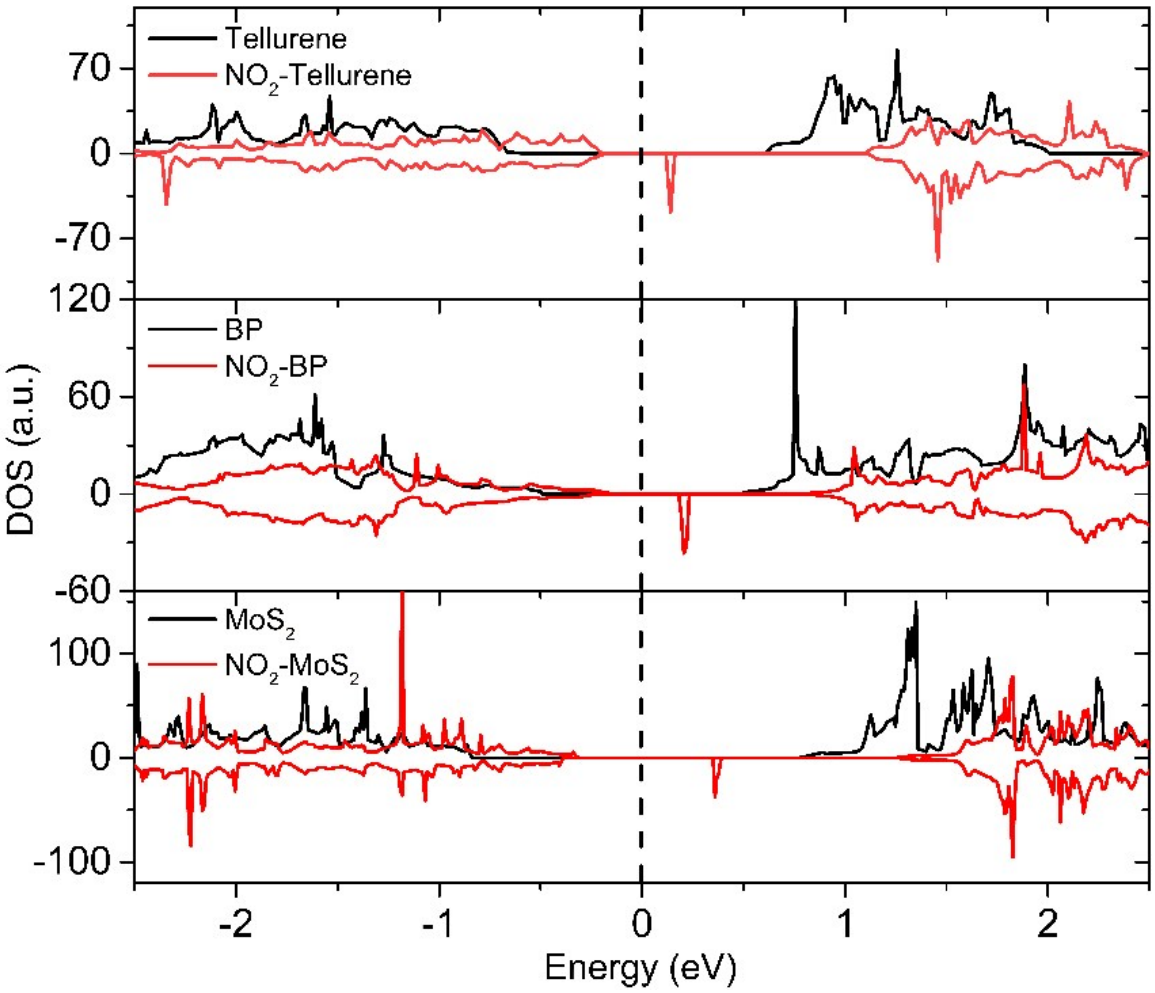

Figure S7. The density of states (DOS) of NO_2 adsorption on tellurene, phosphorene (BP), and MoS_2.

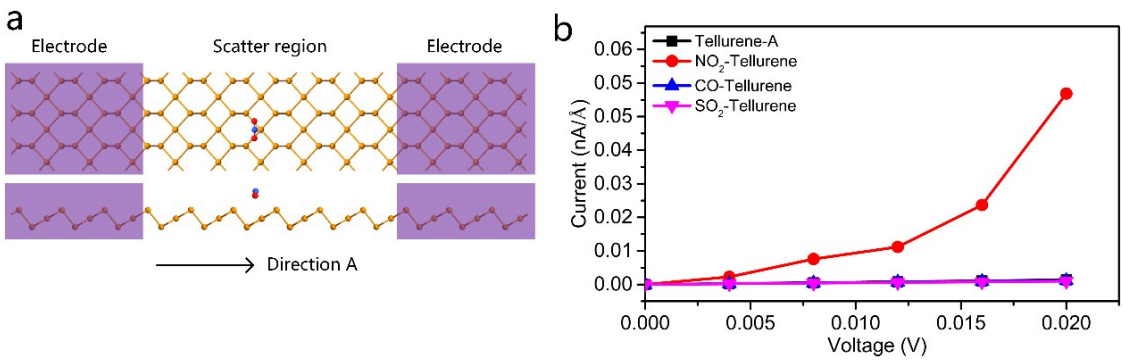

Figure S8. a. The transport model with two probes along the direction A. The purple shaded region represents the electrode region. The electrodes are heavily p-type doped to improve the convergence. **b**. The current-voltage (*I-V*) curves of tellurene with different gas adsorption along the direction A.

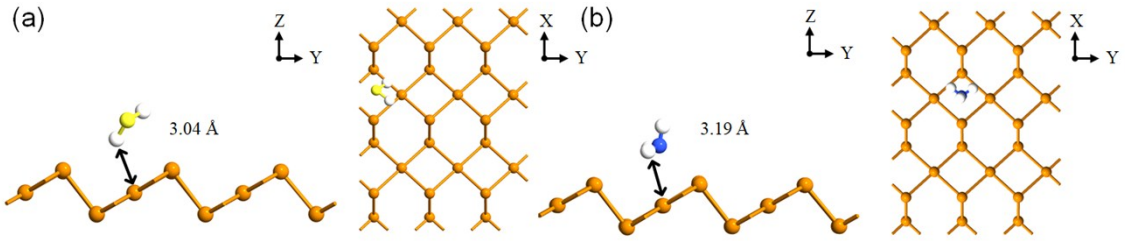

Figure S9. The optimized adsorption structures (front view and top view) of different adsorption systems: a. H_2S adsorption on tellurene. b. NH_3 adsorption on tellurene. The adsorption energies of H_2S and NH_3 adsorption on tellurene are -0.419 eV and -0.521 eV. The charge transfer value are 0.025 e and 0.048 e respectively for H_2S and NH_3.

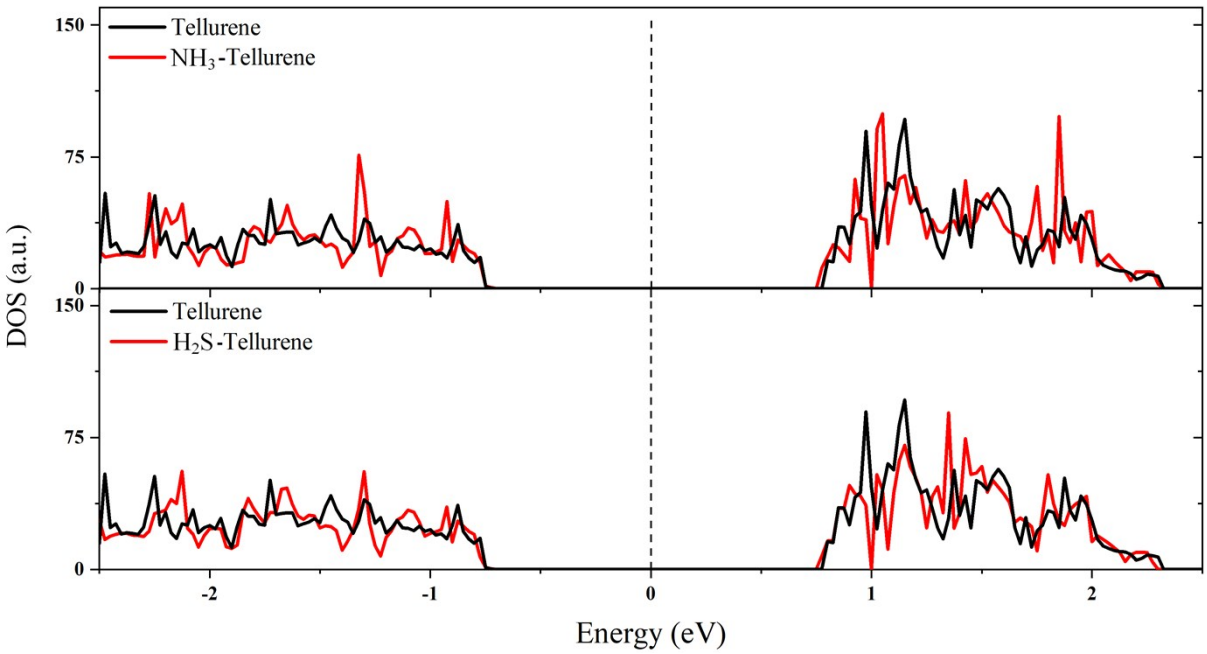

Figure S10. The density of states (DOS) of NH_3 and H_2S adsorption on tellurene.

References:

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