Supporting Information

Fabrication of 1D Te and 2D ReS_2 Mixed-Dimensional van der Waals *p-n* Heterojunction for High-Performance Photodetector

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Experimental Methods

Photodetector Device Fabrication.

The Te NWs were separated using high-speed centrifugation and then was rinsed with absolute alcohol and acetone three times. Then, these nanowires were dispersed in alcohol for the next step of composition. The Te NWs, which are dispersed in ethanol, are dropped onto SiO_2/p^+-Si substrate and then dried naturally. Then the ReS_2 NFs were mechanically exfoliated from the bulk crystals (the bulk ReS_2 was commercially available from Six Carbon Technology Supplies) onto the SiO_2/p^+-Si substrate by using the "Scotch-tape" method. The ReS_2 NFs with 7.9 nm thickness and proper lateral size were selected for device fabrication. Then, a dry-transfer technique was employed to fabricate the Te/ReS_2 heterojunction onto SiO_2/p^+-Si substrate. In detail, the Te NWs transfer processes were carried out using a polydimethylsiloxane (PDMS) coated propylene carbonate (PPC). When heated to 60 ℃, the PDMS and PCC will separate, the Te NWs will adhere to the PCC. Then, the PPC coated Te NWs was transfer onto the ReS_2 NFs. After the transfer, the PPC was eliminated by acetone and cleaned by isopropanol. We made the patterns of source and drain by standard electron beam lithography. A layer of 10/70 nm Cr/Au was then deposited by sputtering. Finally, the lift-off process was taken for the metal contacts.

Density Functional Theory (DFT) Calculations.

First, for ReS_2, we constructed a 2 × 2 supercell containing 4 Re and 8 S atoms to calculate the band structure of pristine ReS_2. A vacuum layer of 15 Å is placed above the monolayer to avoid the interaction between the adjacent layers, and a cut off energy of 500 eV and a precise 9 × 9 × 1 k-point sampling grid are used. All of the atoms in the supercell are allowed to relax until residual forces have converged to less than 2.0×10^{-3} eV/Å and the total energy to less than 1.0×10^{-4} eV during the structural optimization.[1] Then, for the properties of Te, the Heyd - Scuserian - Ernzerhorf (HSE06) hybrid functional[2] was used in order to obtain an accurate band gap in monolayer (1 L) and bulk Te because this functional is computational and machine demanding. The cut off energy plane-wave basis was set to be 500 eV. The vacuum space vertically along the *z*-direction was set to over 16 Å in to mimic the 2D system and to avoid the interaction between layers and its periodic images. During optimization and single point calculations, vdW interaction is considered in PBE exchange functional proposed by Grimme (DFT-D2)[2] to account for the inter-layers' interaction in few-layer Te (layer number (L) > 1). The atomic positions were fully relaxed until the forces on all atoms were less than 10^{-2} eV/Å. The energy convergence criterion was set to be 10^{-6} eV/cell using the Fast (Davison and RMM-DIIS) algorithm. A dense k-mesh of 15 × 15 × 1 sampling with the Monkhorse-Pack scheme[4] was used for both optimization and single point calculation in the Brillouin zone integration.

REFERENCES

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(2) Heyd, J.; Scuseria, G.E. Assessment and validation of a screened Coulomb hybrid density functional. *J. Chem. Phys.* **2004**, *120*, 7274-7280.

(3) Perdew, J.P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1997**, *78*, 1396.

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Fig. S1 Schematic for the fabrication process of Te, ReS_2, and Te/ReS_2 FET based phototransistors.

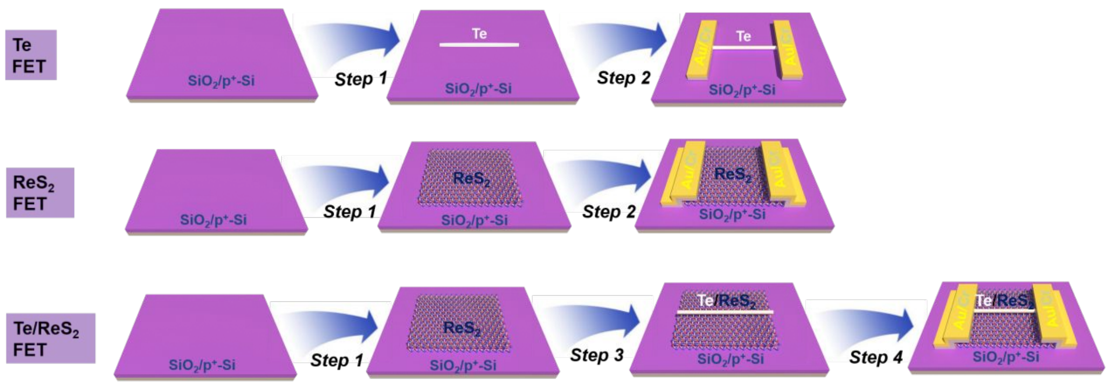


Fig. S2 The SEM and optical microscope images of (a) ReS_2 and (b) Te/ReS_2 mixed dimensional heterjunction devices.

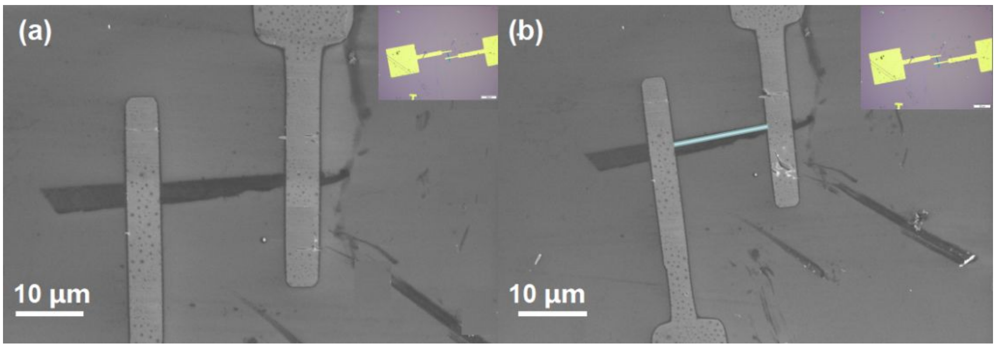


Fig. S3 The I_{ds}-V_d curves at V_g of 0 V of (a) Te, (b) ReS_2, and (c) Te/ReS_2 devices.

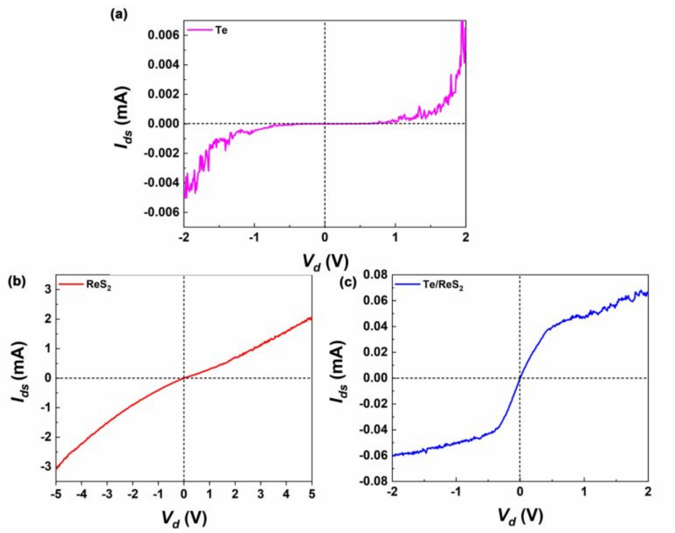
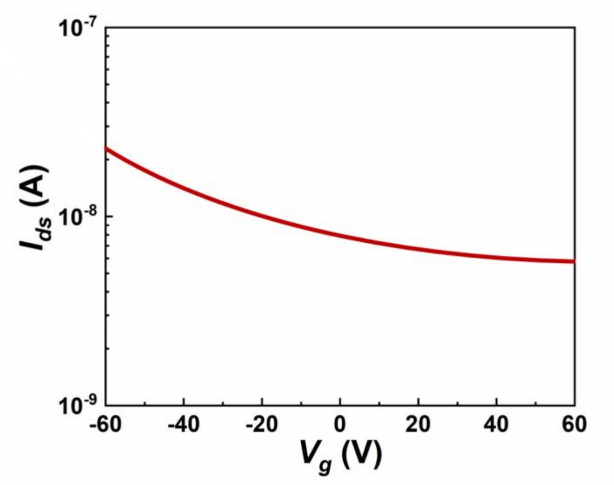


Fig. S4 Transfer curve of Te FET measured under dark at V_{ds} = 1 V.



The transfer characteristic of Te is demonstrated in Fig. S4 and a conspicuous *p*-type behavior was observed under dark. The Te-based FET showed poor performance with low on/off ratio of about 10.

Fig. S5 The V_g-I_{ds} characteristics of (a) ReS_2 and (b) Te/ReS_2 devices at different light intensity with the wavelength of 632 nm.

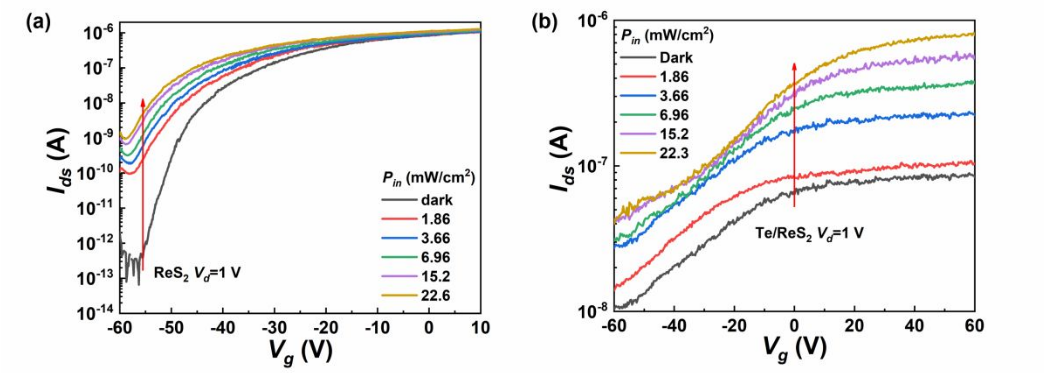


Fig. S6 The I_d-V_d of pure Te device under dark conditions and at maximum light intensity of 22.6 mW/cm^2 with the wavelength of 632 nm.

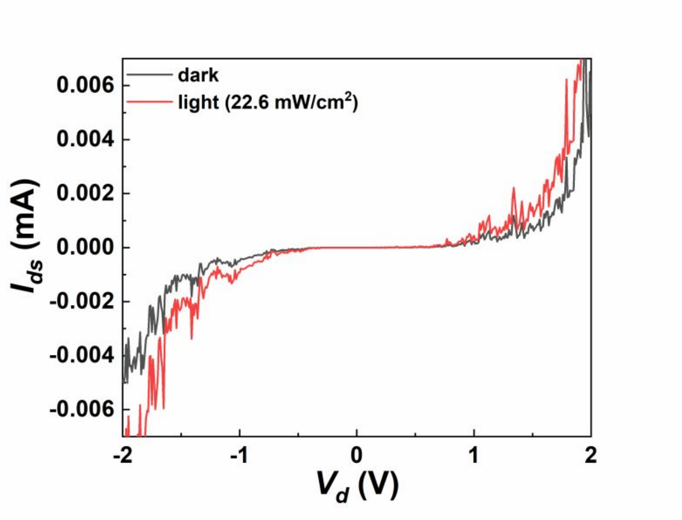


Fig. S6 depicts optoelectronic properties of Te NWs device, exhibiting non-obvious response under 22.6 mW·cm^{-2} illumination.