Synthesis of 2D ternary layered manganese phosphorous trichalcogenides towards ultraviolet photodetection

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ABSTRACT Manganese phosphorous selenium (MnPSe₃), as a representative of layered metal phosphorus trichalcogenides (MPTs), has gained significant attention due to its direct bandgap, high carrier mobility, large absorption coefficient, which indicate great potential in photoelectric application. Herein, high-quality two-dimensional (2D) MnPSe₃ flakes were mechanically exfoliated from the corresponding bulk crystals synthesized by chemical vapor transport (CVT) methods. The systematic investigation was applied to the lattice vibrations of MnPSe₃ via angle-resolved polarized Raman spectroscopy (ARPRS), and the Raman vibration modes were determined based on Raman selection rules and crystal symmetry. Impressively, the photodetectors based on 2D MnPSe₃ flakes exhibit excellent photoresponse to the ultraviolet light with a responsivity up to 22.7 A W⁻¹ and a detectivity of 2.4 × 10¹¹ Jones. The high performance in the ultraviolet range signifies that 2D MnPSe₃ is expected to be a powerful candidate for future ultraviolet photodetection.

Keywords: 2D materials, MnPSe₃, ternary materials, ultraviolet photodetection, phosphorus trichalcogenides

INTRODUCTION

Atomically thin two-dimensional (2D) materials have recently generated widespread interest and shown versatile applications in next-generation optoelectronic, spintronic, and energy devices, owing to their unique structure, mechanical flexibility, and exceptional physical properties [1–3]. Among these materials, 2D metal phosphorus trichalcogenides (MPTs) have emerged as rising stars in numerous fields due to their rich varieties, large bandgaps, and various magnetism orders [4–6]. MPT family include a variety of metal phases (MnPSe₃,

FePSe₃, CdPSe₃, etc.), and bimetal phases (AgVP₂Se₆, CuInP₂S₆, etc.), thus resulting in a large number of components [7]. Interestingly, the variation of metal ions and atomic ratios may lead to tremendous changes in their magnetic states and optical bandgap (from 1.3 to 3.5 eV) [8]. 2D MPTs exhibit larger bandgaps than current 2D transition metal chalcogenides (TMDs), which satisfies the application demands in the broad wavelength response [9]. Accordingly, 2D MPTs are supposed to provide appealing prospects in photodetection, catalysis, and spintronic devices, and expected to be a powerful candidate of next-generation electronics [10–12].

Among MPTs, 2D MnPSe₃ is considered as a promising direct-bandgap semiconductor possessing the structure of the [P₂Se₆]^{4−} cluster surrounded with a honeycomb arrangement of manganese cations [9]. The direct bandgap feature may originate from the manganese cations and the strong ionic bond between Mn cations and [P₂Se₆]^{4−} endows MnPSe₃ with a comparatively large bandgap [13]. Very recently, it was theoretically predicted that 2D MnPSe₃ owns higher carrier mobility (about 625.9 cm² V^{−1} s^{−1}) and larger absorption coefficient (2 × 10⁵ cm^{−1}) than other MPT counterparts, which provides extraordinary opportunities for novel applications in optoelectronics at ultraviolet wavelengths [9,14]. However, the current experimental research for 2D MnPSe₃ primarily focuses on catalytic activity in photocatalysis and electrocatalysis [15]. Most of the reported 2D MnPSe₃ were prepared by the liquid-phase exfoliation method which hinders the applications in optoelectronics due to their poor crystallinity and unclean surface [16]. According to the fascinating properties mentioned above, it is extremely urgent to promote further exploration of

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the optoelectrical properties based on high-quality 2D MnPSe₃ crystals.

In the present work, high-quality 2D MnPSe₃ crystals are successfully isolated *via* a mechanical exfoliation method from the bulk crystals synthesized by the chemical vapor transport (CVT) method. A systematic investigation by angle- and temperature-dependent Raman spectroscopy for the first time reveals the lattice vibration and interlayer coupling of 2D MnPSe₃ flakes. Also, the optoelectrical properties have been systematically investigated and the photodetectors based on 2D MnPSe₃ flakes display excellent performance in the ultraviolet range with a high responsivity of 22.7 A W⁻¹ and detectivity of 2.4×10¹¹ Jones. The high performance of 2D MnPSe₃-based ultraviolet photodetector paves the way for promising applications in optoelectronics.

EXPERIMENTAL SECTION

Material preparation

High-quality MnPSe₃ single crystals were synthesized *via* the CVT method (Fig. S1). Manganese powder (99.95%, Alfa), phosphorus powder (99.9% Alfa), and selenium powder (99.9% Aladdin) were stoichiometrically mixed (1:1:3) together with iodine as the transport agent and sealed into an evacuated quartz tube under vacuum (10⁻⁴ torr). Whereafter, the tube was placed in a two-zone horizontal furnace with the hot end at 993 K and cold end at 893 K. After 7 days, the furnace was cooled naturally to room temperature and rufous plate-like MnPSe₃ single crystals were obtained. The 2D MnPSe₃ flakes were achieved on the SiO₂/Si substrate by the mechanical exfoliation method (Fig. S2).

Characterization

The MnPSe₃ single crystals were characterized by a powder X-ray diffractometer (XRD, XRD D2 PHASER, Bruker). The MnPSe₃ flakes were characterized and identified by an optical microscope (OM, OM BX53M, Olympus), an atomic force microscope (AFM, AFM Dimension Icon, Bruker), a transmission electron microscope (TEM, TEM Tecnai G2 F20, FEI), an X-ray photoelectron spectrometer (XPS, XPS AXIS-ULTRA DLD-600 W, Kratos), a Raman microscope (Raman Alpha 300 RS+, WITec) and a microspectrophotometer (MSV 5200, Jasco).

Device fabrication and electrical property measurement

The electrical device based on MnPSe₃ flakes was fabricated by electron-beam lithography (Quantum FEG 650

scanning electron microscope and Raith Elphy Plus) and Cr/Au (10 nm/90 nm) electrodes were deposited by thermal evaporation (Nexdep, Angstrom Engineering). The temperature-dependent electrical property was characterized under vacuum of 5×10⁻⁶ Pa by a cryogenic probe station (CRX-6.5 K, Lakeshore) connecting to a Keithley semiconductor measurement system (4200SCS, Keithley). The photoelectric measurement was performed under a laser-driven illuminant (EQ-1500, Energetiq).

RESULTS AND DISCUSSION

The MnPSe₃ crystallizes into the rhombohedral structure of space group $R\bar{3}$ (No. 148) with $a = b = 0.6387$ nm, $c = 1.9996$ nm. As shown in Fig. 1a, the crystal structure can be viewed as the stacking of sandwich-like SeMn_{2/3}(P₂)_{1/3}Se slabs bonded by van der Waals interaction with an interlayer spacing of ~0.67 nm [15,17]. The van der Waals layers are shifted so that each phosphorus dimer is sandwiched between two metal atoms in the adjacent layers (the rectangular region in Fig. 1a) [18]. The top view of MnPSe₃ (Fig. 1b) exhibits the honeycomb arrangement of six Mn cations surrounding one phosphorus atom [19]. Within the layer, each MnPSe₃ unit cell is made up of two Mn²⁺ ions and one [P₂Se₆]⁴⁻ cluster which is formed by a dumbbell-like P dimer bonded to six selenium atoms [17]. In particular, the strong ionic bond between Mn²⁺ and [P₂Se₆]⁴⁻ cluster contributes to the comparatively large bandgap [9]. In Fig. 1c, the MnPSe₃ can be regarded as the combination of two distinct atomic groups, MnSe₆ and P₂Se₆, both of which exhibit near-octahedral coordination [18]. The MnPSe₃ single crystals synthesized by the CVT method were characterized by XRD which exhibits distinct sharp peaks and matches well with the standard MnPSe₃ pattern (PDF#89-1414), indicating the high crystalline quality and phase purity of the as-synthesized MnPSe₃ crystals (the inset in Fig. 1d). Besides, only (0 0 1) peaks in the XRD pattern suggest that the crystals have a high prior orientation along the *c*-axis. Thanks to the low cleavage energy of MnPSe₃ crystals which indicates weak interlayer van der Waals interactions and feasibility of exfoliation, we achieved few-layer MnPSe₃ flakes on 300-nm-thick SiO₂/Si substrate (Fig. 1e) by using the scotch tape exfoliation method and demonstrated its smooth and flat surface with a thickness of ~1.5 nm which corresponds to the thickness of two van der Waals layers (Fig. 1f) [20]. Moreover, XPS was performed to characterize the chemical states of the synthesized MnPSe₃ (Fig. 1g-i). The fitting curves of Mn 2p located at around 652.6 and 639.8 eV can be assigned to Mn 2p_{1/2} and Mn 2p_{3/2}. The

Figure 1 Structure and characterizations of 2D MnPSe₃ flakes. (a) Front view and (b) top view of few-layer MnPSe₃. (c) Detailed structure images of MnSe₆ and P₂Se₆. (d) XRD pattern of the MnPSe₃ single crystal; the inset shows the image of a typical MnPSe₃ crystal. (e) OM and (f) AFM images of the exfoliated MnPSe₃ flakes. XPS patterns of (g) Mn 2p, (h) P 2p, and (i) Se 2p.

Se 3d spectrum displays two peaks at 54.5 and 53.7 eV which are related to Se 3d_{3/2} and Se 3d_{5/2}. Two peaks at 131.8 and 130.9 eV in the P 2p spectrum are attributed to P 2p_{1/2} and P 2p_{3/2}, whereas the third peak centered at 138.2 eV is related to the combination of P 2p level surface and Se Auger emission line [21]. All the peaks mentioned above are in agreement with the experimental values reported previously [15].

To demonstrate the crystal structure, crystallinity, and elemental homogeneity of the 2D MnPSe₃ crystals, TEM was utilized to character the exfoliated flake. The low-magnification TEM image of 2D MnPSe₃ flake is shown in Fig. 2a and the diaphanous nature confirms its ultrathin thickness. The obtained high-resolution TEM (HRTEM) image displays distinct clear fringes with spacing of 0.18 nm which is in good accordance with (300) plane (Fig. 2b). The selected area electron diffraction (SAED) image (Fig. 2c) with distinct hexagonal diffraction spots verifies the single-crystalline nature of the ex-

foliated 2D MnPSe₃ flake and the elemental mapping images of Mn, P, and Se elements are shown in Fig. 2d–f, which indicate a uniform distribution of elements and high-quality nature. The energy-dispersive X-ray spectroscopy (Fig. S3a, b) shows the elemental ratio of Mn, P, and Se close to 1:1:3, corresponding to the stoichiometric ratio of MnPSe₃.

Raman spectroscopy has proven to be a fast and non-destructive technique in the characterization of crystal structure, vibration mode, and interlayer coupling [22]. The angle-resolved polarized Raman spectroscopy (ARPRS) was employed to determine the Raman vibration modes based on Raman selection rules and crystal symmetry [23]. The schematic view of the polarized Raman configurations is depicted in Fig. 3a, where the incident laser polarized direction is changed by rotating a half-wave plate, and the scattered laser received by the detector is set to a fixed polarized configuration through the polarizer, while the sample is kept motionless. Non-polarized,

Figure 2 TEM analysis of 2D MnPSe_3 flakes. (a) Low-magnification TEM image, (b) HRTEM image, and (c) the corresponding SAED pattern of an exfoliated MnPSe_3 flake. Elemental mapping images of (d) Mn, (e) P, and (f) Se.

Figure 3 Angle-resolved Raman investigation of 2D MnPSe_3 flakes. (a) Schematic view of the polarization Raman configurations. (b) Non-, parallel- and cross-polarization Raman spectra of MnPSe_3 flake. (c) Contour-color map of angle-dependent Raman intensities under parallel polarization configuration. (d) Polar plots of Raman intensity of P_4 and P_5 .

parallel-polarization, and perpendicular-polarization Raman spectra measured at 0° with different intensities of Raman peaks in Fig. 3b show a dependence of polarization. Fig. 3c displays the contour-color plot of angle-de-

pendent Raman intensities under parallel-polarization configuration. The corresponding sample and polarization-dependent Raman spectra are displayed in Fig. S4a, b. The relation between Raman intensity and Raman

mode can be described by the following equation [24]:

$$I \propto \sum_j |e_i \cdot R_j \cdot e_s|^2. \quad (1)$$

Here, e_i and e_s represent the unit polarization vectors of the incident and scattered light, respectively [25]. The incident light polarization e_i can be set as $(\cos\theta \sin\theta \ 0)$, in which θ represents the angle at which the half-wave plate has been rotated. The scattered light polarization e_s is fixed at $(1 \ 0 \ 0)$. The Raman tensors R_j of MnPSe_3 , which belongs to the $R\bar{3}$ space group, can be denoted as:

$$R(A_g) = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & b \end{pmatrix} R(E_g) = \begin{pmatrix} c & d & e \\ d & -c & f \\ e & f & 0 \end{pmatrix}, \begin{pmatrix} d & -c & -f \\ -c & -d & e \\ -f & e & 0 \end{pmatrix}. \quad (2)$$

By substituting e_i , e_s , and R_j into Equation (1), the Raman intensities of A_g and E_g modes are defined as $(a\cos\theta)^2$ and $c^2 + d^2$, respectively, which means the intensity of A_g mode is polarization-dependent but the intensity of E_g mode behaves independently on polarization. Accordingly, the experimental results are in accord with the theoretical curves. P_2 and P_5 peaks can be identified as A_g Raman mode, indicating the out-plane vibration character, whereas P_1 , P_3 , and P_4 are assigned as E_g Raman mode belonging to the in-plane vibration mode (Fig. 3d, Fig. S4c–e) [24]. The analysis data under cross-polarization is displayed in Fig. S5, which is consistent with the results under parallel-polarization.

The Raman spectra of 2D MnPSe_3 flakes with different

thicknesses are shown in Fig. 4a. Among the five Raman peaks we obtained, P_2 , P_3 , P_4 , and P_5 exhibit relatively distinct intensity. Thus Fig. 4b presents the thickness-dependent peak position vibration of these four peaks. The vibration of P_4 varies negligibly with increasing thickness, whereas the other three Raman peaks show a conspicuous thickness-dependent behavior. P_3 and P_5 go through a “red-shift” as the sample thickness increases, while P_2 shows a “blue-shift” trend. Both of the E_{2g}^1 and A_g Raman modes are predicted to behave “blue-shift” due to the enhanced effective reestablished forces acting on the atoms as the thickness increase, based on a classical model for coupled harmonic oscillators [26]. However, the variation of E_{2g}^1 mode is inconsistent with the theoretical prediction. This abnormal trend may be ascribed to the influence of structural changes induced by layer stacking or the long-range Coulombic interlayer interactions [26]. Therefore, the abnormal variation of MnPSe_3 Raman peaks may be caused by the confrontation of several effects mentioned above. Moreover, Raman mappings of two typical peaks P_4 and P_5 assigned to E_g and A_g mode, respectively, are shown in Fig. 4c, demonstrating the homogeneity of MnPSe_3 flake. The Raman mapping of the other three peaks can be found in Fig. S6.

Temperature-dependent Raman measurements (Fig. 5a) were employed to explore the thermal expansion and interlayer coupling of MnPSe_3 flakes. As shown in Fig. 5b, P_2 , P_4 , and P_5 behave a distinct “red-shift” from 80 to 300 K, which can be explained as the change in phonon energies induced by the lattice thermal expansion and

Figure 4 Thickness-dependent Raman measurement. (a) Raman spectra of the MnPSe_3 flake with different layers. (b) Layer-dependent Raman peak position of the MnPSe_3 crystal. (c) Raman mapping images of P_4 and P_5 .

Figure 5 Temperature-dependent Raman measurement. (a) Raman spectra of MnPSe₃ flake at different temperatures ranging from 80 to 300 K. (b) Temperature-dependent Raman peak positions of P₂, P₃, and P₅.

anharmonic phonon coupling [27]. Besides, the linear relationship between the peak position and temperature can be fitted by the following equation:

$$\omega(T) = \omega_0 + \chi T, \quad (3)$$

where ω_0 and χ represent the Raman peak position at 0 K and first-order temperature coefficient, respectively. The χ extracted from the fitting lines of P₂, P₃, and P₅ are $-(0.64 \pm 0.026) \times 10^{-2}$, $-(0.90 \pm 0.037) \times 10^{-2}$, and $-(1.01 \pm 0.019) \times 10^{-2} \text{ cm}^{-1} \text{ K}^{-1}$, respectively, which are smaller than that of other typical 2D materials [28]. As is reported, the first-order temperature coefficient is directly related to the interlayer interaction [29]. For example, the first-order temperature coefficient of SnS ($-3.6 \times 10^{-2} \text{ cm}^{-1} \text{ K}^{-1}$) [30] and SnSe ($-3.8 \times 10^{-2} \text{ cm}^{-1} \text{ K}^{-1}$) [28], which own strong van der Waals interaction, are larger than those of graphene ($-1.6 \times 10^{-2} \text{ cm}^{-1} \text{ K}^{-1}$) [31] and MoS₂ ($-1.1 \times 10^{-2} \text{ cm}^{-1} \text{ K}^{-1}$) [32] with weak interlayer van der Waals interaction. In our case, the calculated cleavage energy of MnPSe₃ is smaller than that of graphite, thus leading to a weak interlayer interaction and relatively small χ , further demonstrating the high flexibility nature of the 2D MnPSe₃ (Fig. S7) [20].

To further investigate the electronic transport behaviors, the temperature-dependent *I-V* measurements of 2D MnPSe₃ are depicted in Fig. 6a, in which the current *I* rises monotonously as the temperature increases from 20 to 300 K, indicating a semiconductor nature of 2D MnPSe₃. Fig. 6b presents the resistance and conductivity extracted from *I-V* curves in Fig. 6a. From 180 to 300 K,

the optical phonons assisting in hopping of small polarons plays a dominant role in the conduction process (Fig. 6c), which can be written as follows:

$$\sigma = \left(\frac{v_0 e^2 c (1-c)}{kTr} \right) \exp \left(-2\alpha r - \frac{\Delta E}{kT} \right), \quad (4)$$

where v_0 represents the frequency of longitudinal optical phonon, c is the fraction of sites occupied by electrons, r is the average of hopping distance, α is the rate of wavefunction decay, and ΔE is the activation energy [33]. ΔE is calculated to be a small value of 109 meV extracted from the fitting curve in Fig. 6c. The small activation energy ensures the minimal fluctuation of ionic conductivity with temperature variation, indicating potential applications of solid electrolytes [34]. When the temperature is below 180 K, as displayed in Fig. 6d, there is an obvious deviation from the fitting curve of Equation (4), which can be well consistent with the variable-range hopping theory put forward by Davis and Mott, as shown in Equation (5):

$$\sigma = \sigma_0 \exp \left[- \left(\frac{T_0}{T} \right)^{1/4} \right], \quad (5)$$

in which σ_0 and T_0 are constants. The contribution of optical phonons to electrical transport decreases as the temperature drops due to the lack of enough energy assisting in hopping, thus leading to the predominance of hopping process assisted by single acoustic phonons at low temperature [35].

To systematically explore the optoelectronic properties of 2D MnPSe₃, we fabricated two-electrode photo-

Figure 6 Electrical properties of the device based on the 2D MnPSe₃ flakes. (a) Temperature-dependent electrical measurements of the 2D MnPSe₃ flakes. (b) The resistance and conductivity as a function of temperature. (c) $\ln(\sigma T) \cdot T^{-1}$ plot from 20 to 300 K and the red line is fitted with an optical phonon hopping model. (d) $\ln(\sigma) \cdot T^{-1/4}$ plot from 20 to 300 K and the red line is fitted with a variable-range hopping model.

detectors based on MnPSe₃ flake, as illustrated in Fig. 7a and the optical microscopy image can be seen in Fig. S8a. As shown in Fig. 7b, the micro-zone UV-vis optical absorption spectrum was employed to demonstrate the bandgap of 2D MnPSe₃ flake on a quartz substrate, and the equation of optical bandgap is presented as follows [36]:

$$\alpha h\nu = A(h\nu - E_g)^m, \quad (6)$$

where α is the absorption coefficient, h is the Planck constant, ν is the light frequency, and m is 1/2 for direct bandgap, while 2 for indirect bandgap. The $(\alpha h\nu)^2$ versus $h\nu$ is plotted in the inset of Fig. 7b and the direct bandgap of MnPSe₃ flake can be confirmed as 2.8 eV from the intercept of the linear part in the low energy region. Fig. 7c shows the normalized I - V characteristics of the photodetector in the dark condition and under different wavelengths of light illumination varied from 300 to 600 nm. It can be seen that a cutoff response wavelength of 400 nm corresponds to the material bandgap (2.8 eV) and the best performance at a wavelength of 300 nm can be associated with the maximum absorption peak around 300 nm in Fig. 7b. As can be seen, the MnPSe₃ photo-

detector shows a prominent response in the ultraviolet range, and thus we measured the current-voltage curves of the photodetector under the illumination of 300 nm with varying power intensity from dark to 713.9 $\mu\text{W cm}^{-2}$, as shown in Fig. 7d. The maximum net photocurrent measured at 713.9 $\mu\text{W cm}^{-2}$ shows the on-off ratio of 8.24. To determine the optoelectrical performance of the 2D MnPSe₃ flake, several essential parameters such as responsivity ($R_\lambda = I_{\text{ph}}/(PS)$, I_{ph} , P , and S represents the photocurrent, power density of light and effective area of $\sim 16 \mu\text{m}^2$) and external quantum efficiency ($\text{EQE} = hcR_\lambda/(e\lambda)$) are introduced to evaluate the sensitivity of the photodetectors [37,38]. In addition, specific detectivity (D^*) is crucial for judging the detection ability of photodetector. D^* can be defined as $D^* = (\Delta f S)^{1/2}/\text{NEP}$, where Δf is the bandwidth, S refers to the effective area and NEP represents the noise equivalent power. The NEP can be calculated as $\text{NEP} = (\bar{i}_n^2)^{1/2}/R$, where $(\bar{i}_n^2)^{1/2}$ can be obtained as the mean-square noise current at the bandwidth of 1 Hz under dark condition from Fig. S9, and the extracted NEP value is $6.37 \times 10^{-14} \text{ A Hz}^{1/2}$ [39]. As shown in Fig. 7e, responsivity,

Figure 7 Device structure and optoelectrical performance. (a) Schematic of the photodetector based on MnPSe₃ flakes. (b) UV-vis optical absorption spectrum of MnPSe₃ flake. The inset is the corresponding fitting curve for optical bandgap. (c) Wavelength-dependent *I*-*V* curves from 300 to 600 nm. (d) *I*-*V* curves in the dark and different power intensities under 300 nm illumination. (e) Responsivity and detectivity deduced from the *I*-*V* curves in (d). (f) Response behavior of the device at *V*_{ds} = 5 V under 300 nm light.

detectivity, and EQE calculated from the photocurrent in Fig. 7d are 22.7 A W⁻¹, 2.4×10¹¹ Jones, and 9400% under the wavelength of 300 nm with 24.2 μW cm⁻² light intensity, respectively. The responsivity of the photodetector based on 2D MnPSe₃ is superior to other typical 2D ultraviolet photodetectors, such as NiPS₃ (0.126 A W⁻¹ @ 254 nm), CuInP₂S₆ (0.01 A W⁻¹ @ 280 nm), GaN (0.15 A W⁻¹ @ 360 nm), and Ga₂O₃ (12.4 A W⁻¹ @ 254 nm) [40–43]. The high ultraviolet detection performance of 2D MnPSe₃ may be attributed to the combination of photoconductive effect and photo-gating effect (Fig. S10) [44]. It is worth noting that the *R*_λ and *D*⁺ reveal a downtrend as light intensity increases in Fig. 7e. At low light intensities, the photo-induced electrons occupy the surface states of 2D MnPSe₃ flake, resulting in a high carrier separation efficiency. With increasing power intensity, the surface trap states will be occupied quickly due to a mass of photo-generated electrons, and until the trap states are totally occupied, the photo-generated electrons and holes will recombine immediately and not participate in the charge transfer process, thus leading to the downward trend of *R*_λ and *D*⁺ [45,46]. Fig. 7f proves the stability of the time-resolved photocurrent curves measured by switching the incident 300 nm light @ 713.9 μW cm⁻² on/off with a time interval of 5 s under a bias voltage of 5 V. The response time can

be defined as the required time for increasing from 10% to 90% of peak values, and thus the rising and decay times are calculated to be 470 ms and 1.8 s, respectively, as displayed in Fig. S8b. These excellent ultraviolet detection capabilities make few-layer ternary MnPSe₃ a powerful competitive candidate for prospective ultraviolet detection.

CONCLUSIONS

In conclusion, we successfully isolated high-quality 2D MnPSe₃ flakes from the corresponding bulk crystals synthesized by the CVT method. Systematical Raman investigations were performed for MnPSe₃ flakes to assign Raman modes and the variation of peak positions with thickness and temperature. Furthermore, we for the first time introduced MnPSe₃ to the photoelectrical 2D materials family. The photodetectors based on 2D MnPSe₃ flakes display excellent performance in the ultraviolet range with a high responsivity of 22.7 A W⁻¹ and detectivity of 2.4×10¹¹ Jones. All these results indicate that 2D ternary MnPSe₃ is prospective for the next-generation optoelectronics.

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Author contributions Liu G conceived the experiments and synthesized the MnPSe_3 . Liu G and Su J carried out the characterization of MnPSe_3 . Liu G and Feng X did the Raman measurement. Liu G and Su J performed the photoelectrical measurement and wrote the manuscript under the guidance from Li H and Zhai T. All the authors contributed to the experimental planning and discussions.

Conflict of interest The authors declare no conflict of interest.

Supplementary information Experimental details and supporting data are available in the online version of the paper.

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二维层状 MnPSe_3 的合成及紫外光探测应用

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摘要 作为层状金属磷硫属化合物的典型代表, MnPSe_3 以其直接带隙特性、高载流子迁移率以及大的吸收系数而备受关注, 在光电领域展现了巨大潜力. 本文中, 我们对化学气相输运法制备的单晶进行机械剥离从而获得了高质量的二维 MnPSe_3 纳米片, 利用角分辨偏振拉曼光谱对 MnPSe_3 的晶格振动进行了系统的研究, 并根据拉曼选择定则和晶体的对称性确定了其拉曼振动模式. 我们构建的基于二维 MnPSe_3 纳米片的光电探测器对紫外光的响应度和探测度分别高达 22.7 A W^{-1} 和 $2.4 \times 10^{11} \text{ Jones}$. 在紫外区域优异的探测能力表明二维 MnPSe_3 有望应用于未来紫外光电探测领域.