High-Performance Few-layer Mo-doped ReSe\(_2\) Nanosheet Photodetectors

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Transition metal dichalcogenides (TMDCs) have recently been the focus of extensive research activity owing to their fascinating physical properties. As a new member of TMDCs, Mo doped ReSe\(_2\) (Mo:ReSe\(_2\)) is an octahedral structure semiconductor being optically biaxial and highly anisotropic, different from most of hexagonal layered TMDCs with optically uniaxial and relatively high crystal symmetry. We investigated the effects of physisorption of gas molecule on the few-layer Mo:ReSe\(_2\) nanosheet based photodetectors. We compared the photoresponse of the as-exfoliated device with annealed device both in air or ammonia (NH\(_3\)) environment. After annealing at sub-decomposition temperatures, the Mo:ReSe\(_2\) photodetectors show a better photoresponsivity (\(\sim 55.5\) A/W) and higher EQE (10893%) in NH\(_3\) than in air. By theoretical investigation, we conclude that the physisorption of NH\(_3\) molecule on Mo:ReSe\(_2\) monolayer can cause the charge transfer between NH\(_3\) molecule and Mo:ReSe\(_2\) monolayer, increasing the n-type carrier density of Mo:ReSe\(_2\) monolayer. The prompt photoswitching, high photoresponsivity and different sensitivity to surrounding environment from the few-layer anisotropic Mo:ReSe\(_2\) can be used to design multifunctional optoelectronic and sensing devices.

Two-dimensional (2D) materials are an emerging class of new materials with exotic properties and great promise for use in next-generation nanoelectronic devices. The most studied 2D materials, graphene, has shown exceptional physical, chemical, optical, magnetic and mechanical properties\(^1\)–\(^7\). Graphene-based optoelectronic devices not only operate in a very wide wavelength range\(^8\)–\(^9\), but also show extremely fast carrier transport (approaching ca. 20 0000 cm\(^2\) V\(^{-1}\) s\(^{-1}\) for a free sheet)\(^2\)–\(^10\). Despite graphene’s superior properties, graphene is a zero-gap semimetal, and the lack of optical band gap limits its applications\(^11\). Therefore, the research based on other 2D materials with an intrinsic band-gap has been triggered.

Photodetector is an optoelectronic device that absorbs light with a certain wavelength and generates electron-hole pairs, and then produces electrical signal due to separation and directional movement of the electron-hole pairs. In recent years, photodetectors have made remarkable progress driven by urgent needs in numerous applications, such as flame detection, engine monitoring, missile plume detection, chemical/biological sensing, and intersatellite communications\(^15\)–\(^17\). It is now widely recognized that nanostructured semiconductors, in comparison to bulk materials, may provide better photodetection performance due to their large surface area, low dimensions and size dependent properties, such as increased photon absorption, enhanced charge separation and migration, and surface sensitivities\(^18\)–\(^19\). Some one-dimensional (1D) semiconducting nanostructures have been utilized to design photodetectors, but preparation of these 1D nanomaterials is usually complex\(^20\). 2D materials are relatively easy to fabricate circuits and some complex structures. The very high surface-to-volume ratio of single- or few-layer 2D materials enables promoted charge separation and highly light sensitivity. Graphene recently has been used for fabricating photodetectors\(^21\). However, graphene-based photodetectors are limited by their low responsivity (\(\sim 10^{-2}\) A/W\(^{-1}\)), low external quantum efficiency (EQE) (0.1–0.2%), and lack of spectral selectivity\(^20\)–\(^22\). Therefore, other 2D materials have been explored for enhancing responsivity and spectral selectivity of photodetectors. Very recently, semiconducting TMDCs with the common formula MX\(_2\), where M indicates a transition metal (M = Mo, W, V, Nb, Ta, Ti, Zr, Hf, Re) and X represents a chalcogen (Se, S or Te), emerged with great research interests\(^23\). GaS nanosheet photodetectors made on SiO\(_2\)/Si substrates or flexible polyethylene terephthalate (PET) substrates exhibit a photoresponsivity at 254 nm of up to 4.2 A/W\(^{-1}\) and 19.2 A/W\(^{-1}\), respectively, which far exceeds that of graphene-based devices. The reduction of the effective mass at the valence band maximum with decreasing layer thickness enhances the carrier mobility of the GaS nanosheets, contributing to the high photocurrent\(^20\). An ultrasensitive monolayer MoS\(_2\) phototransistor shows
a maximum external photoresponsivity of 880 AW⁻¹ at the wavelength of 561 nm. This is due to their improved mobility, as well as the contact quality and positioning technique²³.

Most of the 2D layered materials, such as graphene, MoS₂, WS₂ and WSe₂ et al. have highly crystal symmetry. Therefore, the photonic, electronic, and mechanical properties of these 2D materials are largely isotropic and almost do not depend on the change of direction. In fact, the anisotropic properties of 2D materials have rarely been explored before for novel optoelectronic and electronic device applications. Mo:ReSe₂, a new member of TMDCs, is an anisotropic semiconductor crystallized in a distorted layered CdCl₂-type octahedral structure of triclinic symmetry, different from most of hexagonal layered TMDCs. A clustering of Re₄ diamond units forms along the b-axis within the van der Waals plane in Mo:ReSe₂ monolayer, resulting in the crystals being optically biaxial²⁴. However, other TMDCs with hexagonal structure (e.g. 2H–MoS₂ and MoSe₂) are optically uniaxial with their optical axis perpendicular to the van der Waals plane²⁵. On account of “diamond chains” clustering structure, Mo:ReSe₂ shows in-plane optical and electrical anisotropic response, which may be exploited for fabrication of polarization sensitive photodetectors, photoelectrochemical solar cells and other optoelectronic devices²⁶,²⁷.

In this communication, we report the few-layer Mo:ReSe₂ nanosheets based photodetectors. These few-layer Mo:ReSe₂ nanosheets were mechanically exfoliated on SiO₂/Si substrates, and were characterized by atomic force microscopy (AFM) and Raman spectra. Two-terminal photodetectors were fabricated with deposition of Au electrodes. We compare the photoresponse of the as-exfoliated devices with annealed devices both in air or NH₃ environment. After annealing at sub-decomposition temperatures, the Mo:ReSe₂ photodetectors show a better photoresponsivity and higher EQE. Especially, the devices operated in NH₃ show higher performance than in air. The response time of device is also less than 100 ms. The prompt photoswitching, high photoresponsivity and different sensitivity to surrounding environment from the anisotropic Mo:ReSe₂ nanomaterials pave an avenue to multifunctional optoelectronic and sensing device applications with 2D semiconductors.

Results

Figure 1a shows the structure of a single layer of Mo:ReSe₂ nanosheet. The 1T-Mo:ReSe₂ consists of edge-shared MX₆ octahedra. The movement of the Re atoms toward each other forms a Re₄ diamond unit which is coplanar and coupled with one another to comprise a clustering pattern of diamond chains, resulting in a lattice distortion²⁴. The layer thickness of Mo:ReSe₂ is ~6.63 Å (Figure 1b). Due to the reduced crystal symmetry, Mo:ReSe₂ displays a more complex Raman spectrum than conventional TMDCs. In Figure 1c the Raman spectrum displays at least eleven Raman modes in the 100–300 cm⁻¹ range, which is significantly more compared to other TMDCs with higher crystal symmetries. And exfoliated few-layer nanosheet has shown characteristic A₁g (out-of-plane) and E₂g (in-plane) Raman modes located at 243 and 284 cm⁻¹ for MoSe₂, which proves the existence of Mo element. The few-layer Mo:ReSe₂
nanosheets prepared by mechanical exfoliation are characterized by AFM. The thickness of these Mo:ReSe2 flakes is mainly in the range of 4–5 nm, which corresponds to a layer number of 7–8 (shown in Figure 1d). The energy-dispersive x-ray (EDX) is used to analyze the composition of the few-layer nanosheets, as shown in the Supporting Information (Figure S1).

Two Au electrodes were made onto the few-layer Mo:ReSe2 nanosheet with a 28 μm wide channel. Monochromatic light (633 nm) was vertically irradiated onto the device (depicted in Figure 2a). Figure 2b shows the photocurrent measured as a function of time (I-t curves) when the photodetectors are illuminated with irradiance of 20 mW/cm² under different conditions (the bias voltage between two electrodes is kept constant at 1 V), (d) multiple cycle operation of the device, (e) and (f) the photocurrent responses with time in the annealed photodetectors under illumination of 633 nm in NH3 environment.

Figure 2 | (a) Schematic of the device operation, (b) I-t curves and (c) I-V curves when the photodetector is illuminated with 633 nm light at an irradiance of 20 mW/cm² under different conditions (the bias voltage between two electrodes is kept constant at 1 V), (d) multiple cycle operation of the device, (e) and (f) the photocurrent responses with time in the annealed photodetectors under illumination of 633 nm in NH3 environment.
that the as-exfoliated Mo₆ReSe₂ shows less sensitive to NH₃ environment. As shown in Figure 2b, the photocurrent of the device increases to \( \sim 0.5 \mu A \) during exposure to NH₃ environment, the photocurrent of the annealed device becomes extremely sensitive to gas environment. As shown in Figure 2b, the photocurrent of the annealed device measured in air decreases by \( \sim 0.5 \mu A \). During exposure to NH₃ environment, the photocurrent of the annealed device increases to \( \sim 4 \mu A \), and the photoswitch ratio is about 20. Compared to the as-exfoliated ReSe₂, the photoswitch ratio of the annealed Mo₆ReSe₂ is enhanced in NH₃ environment. Current-voltage (I–V) characteristics measured in dark or under light illumination are shown in Figure 2c. All I–V curves both in dark and under light illumination are nearly linear, which indicates an Ohmic contact. In the dark, the I–V curve of as-exfoliated device is slightly different from annealed device. Under the light illumination, the photocurrent rises almost instantaneously. In addition, the annealed device exhibits a higher photocurrent when exposed in NH₃ environment. Figure 2d shows the photocurrent switching of the device in NH₃. Each photoresponse cycle consists of three transient regimes: sharp rise, steady state, and sharp decay. As shown in Figure 2d, the current of the device exhibits a low-current state of 0.2 mA in the dark and a high-current state of \( \sim 4 \mu A \) under light illumination. After many cycles, the photocurrent still responds in a similar fashion to the light, which exhibits excellent operation reversibility and stability.

The spectrum responsivity (Rₛ) and EQE are two critical parameters to determine the sensitivity for an optoelectronic device, which represent the ability to provide photo-generated carriers per single incident photon. Rₛ and EQE can be expressed as \( Rₛ = AI/PS \) and \( EQE = t_{light}/t_{trans} = h\epsilon Rₛ/(eλ)\ell \), respectively; \( AI \) is the difference between the current under photoexcitation and the dark current; \( P \) is the light power intensity irradiated on the device (\( P = 20 \text{ mW/cm}^2 \)); and \( S \) is the effective irradiated area of the device (\( S = 336 \mu \text{m}^2 \)). From our experimental results, under an illumination of 635 nm at 1 V (calculated from Figure 2d), the \( Rₛ \) and EQE are calculated to be \( \sim 55.5 \text{ AW}^{-1} \) and \( \sim 10893\% \), respectively. Therefore, these photodetectors show a much better photoresponse compared to most other optoelectronic devices, as shown in Supporting Information Table 1.

The time response speed is also a key factor for photodetectors and it determines the capability of a photodetector to follow a fast-changing optical signal. Response times for photocurrent rise and decay obtained from 1D nanostructures based photodetectors range from seconds to several tens of minutes. Figure 2e and 2f show the photocurrent responses in the annealed device under the illumination (633 nm) in NH₃ environment. The dynamic response to the light illumination for rise and decay in our devices can be expressed by \( I(t) = I_0 [1 - \exp(-t/t_r)] \) and \( I(t) = I_0 \exp(-t/t_d) \), where \( t_r \) and \( t_d \) are the time constants for the rise and decay, respectively. The rise time (decay time) is defined as the time interval for the response to rise (decay) from 10 to 90% (90 to 10%) of its peak value. The time constant \( t_r \) and \( t_d \) are calculated to be 96 ms and 340 ms, respectively, from our device.

**Discussion**

In order to understand the experimental results, first-principles calculations are performed to investigate the adsorption of NH₃ molecule on the Mo₆ReSe₂ surface. A 4 × 4 supercell of Mo₆ReSe₂ monolayer with a single NH₃ molecule adsorbed to it is built for the calculation. The calculated adsorption energy curve for NH₃ in Figure 3a shows that the interaction between the NH₃ molecule and Mo₆ReSe₂ monolayer can be characterized as physisorption due to the small adsorption energy and large separation distance. At equilibrium, the adsorption energy and separation distance are found to be \( \sim -203 \text{ meV} \) and 2.34 Å, respectively. The charge transfer between NH₃ molecule and Mo₆ReSe₂ monolayer is then determined by using the Bader analysis method. It is found that NH₃ molecule behaves as a donor, and donates approximately 0.024 electrons (per supercell) to the underlying Mo₆ReSe₂ monolayer, depleting the charge on NH₃ molecule, as shown in Figure 3b. Since the mechanically exfoliated Mo₆ReSe₂ nanosheet is a n-type semiconductor with background free electrons coming probably from defects (as shown in Supporting Information Figure S3), the adsorption of NH₃ further transfers electrons to the nanosheet and increases its carrier density. Point defects in 2D materials can trap free charge carriers and localize excitons. The charge transfer value can be enlarged if the adsorption of NH₃ molecule occurs at a defect site induced by the experimental annealing. For instance, when NH₃ is adsorption at a single Se vacancy, a larger value of 0.049 electrons can be transferred from the NH₃ molecule to the monolayer Mo₆ReSe₂.
photocurrent was quick and stable. A theoretical investigation of switches and optoelectronic circuits.

Methods

Crystal growth. Single crystals of the MoReSe 2 were grown using the chemical vapour transport method with Br 2 as a transport agent containing two step growth process, leading to n-type conductivity 31. Prior to the crystal growth, a quartz tube (20 cm length) containing Br 2 (~5 mg cm −2 ), Mo (99.99%), Re (99.99%) and Se (99.99%) was cooled with liquid nitrogen, then evacuated and sealed. After that, the powder was shaken well to achieve uniform mixing. The quartz tube was placed in a two-zone furnace and it pre-reacted at 850 °C for 24 h with the growth zone temperature at 1000 °C to prevent the transport of the product. The furnace was then adjusted to one zone at 1000 °C with another zone at 1060 °C, and was produced the temperature gradient over 2 h. With the temperature varying from 1060 to 1000 °C, a temperature gradient of approximately 2 °C cm −1 over an ampoule length of 20 cm gave optimal conditions for the single-crystal growth of the MoReSe 2. After 360 h crystallization, the furnace was allowed to cool down slowly (40 °C h −1) to about 200 °C. Then the ampoule was taken out and the temperature of the end away from the crystals was dropped to condense the Br 2 vapor. When the ampoule reached room temperature, it was opened and the crystals removed. The crystals were then rinsed with acetone and deionized water.

Mechanical Exfoliation of MoReSe 2. Few-layer MoReSe 2 nanosheets were isolated from bulk MoReSe 2 single crystals and then deposited onto the freshly cleaned Si substrates covered by a 300 nm thick SiO 2 layer using the Scotch tape-based mechanical exfoliation method, which was widely employed for preparation of single-layer graphene sheets 21.

Thermal Annealing. The samples were heated to 400 °C in a 25°C/min rate and the temperature was held at 400 °C for one hour in vacuum. After annealing, the furnace was cooled down to room temperature and the samples were taken out of the furnace.

Photodetector devices were fabricated as follows. The Au electrodes were thermally evaporated by laying a Au wire with micrometer-sized diameter as the mask on MoReSe 2 nanosheet exfoliated on the Si/SiO 2 substrates to obtain a gap between two electrodes. After the deposition of electrodes, the Au wire mask was removed so that the sample in gap area could be exposed. Electrochemical experiments were all performed with a CH166D electrochemical workstation in a conventional three-electrode electrochemical cell.

Raman Spectroscopy. Analysis of the few-layer MoReSe 2 nanosheet by Raman spectroscopy was carried out on a WITec CRM200 confocal Raman microscope system with the excitation line of 532 nm and an air-cooling charge-coupled device (CCD) as the detector (WITec Instruments Corp., Germany).

EDX analysis. EDX was utilized for the estimation the composition of MoReSe 2. The concentration of Mo in the ReSe 2 crystals was shown in supporting information Figure S1.

Computational Methods. First-principles calculations are performed using the Vienna ab initio simulation package (VASP) 32 on the basis of density-functional theory (DFT). The exchange-correlation interaction is treated by the van der Waals density functional (vdW DFT) 33 to describe this adsorption system. Meanwhile, a cutoff energy of 450 eV and a Monkhorst-Pack grid 34 of 5 × 5 × 1 for the Brillouin zone integration are employed. In order to eliminate the interaction between two adjacent MoReSe 2 monolayers, a vacuum layer larger than 15 Å is adopted. The geometric structure is fully relaxed until the Hellmann-Feynman force on each atom is less than 0.02 eV Å −1. By means of Bader analysis 35, charge transfer between MoReSe 2 and NH 3 molecule is obtained. The adsorption energy is defined as

\[ E_a = \text{E}_{\text{MoReSe}_2} + \text{E}_{\text{NH}_3} - \text{E}_{\text{MoReSe}_2 + \text{NH}_3} \]

where \( E_{\text{MoReSe}_2} \) and \( E_{\text{NH}_3} \) are the total energies of molecule adsorbed MoReSe 2 , bare MoReSe 2 and isolated molecule. Negative value of \( E_a \) indicates an exothermic adsorption process. The charge density difference is calculated by the formula

\[ \Delta \rho = \rho_{\text{MoReSe}_2 + \text{NH}_3} - \rho_{\text{MoReSe}_2} - \rho_{\text{NH}_3} \]

where \( \rho_{\text{MoReSe}_2} \), \( \rho_{\text{NH}_3} \) and \( \rho_{\text{MoReSe}_2 + \text{NH}_3} \) are the charge densities of molecule adsorbed MoReSe 2 , bare MoReSe 2 and isolated molecule, respectively.

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**Author contributions**

S.Y. conceived the project. S.Y., S.T., Y.L. and F.L. performed the synthesis and measurements. Q.Y. performed the density functional theory calculations. S.Y. wrote the manuscript. All authors have read the manuscript.

**Additional information**

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