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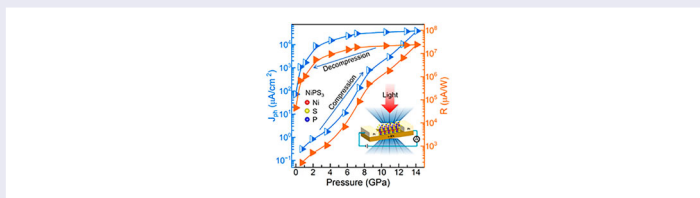
Pressure-induced enhancement and retainability of optoelectronic properties of NiPS₃

Sixue Fang, Quanjun Li, Zonglun Li, Qing Dong, Xiaoling Jing, Chenyi Li, Haiyan Li, Bo Liu, Ran Liu and Bingbing Liu

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ABSTRACT

Here, we report significant pressure-modulate optoelectronic properties of NiPS₃. Upon compression, NiPS₃ exhibited a photocurrent increase of five orders of magnitude over the initial value. Interestingly, when NiPS₃ was finally decompressed to ambient conditions, the photocurrent could maintain a two-order-of-magnitude enhancement. In addition, the spectral response range was extended to the near-infrared spectral range (up to 1650 nm) under high pressure. Raman and XRD measurements and theoretical calculations revealed significant enhancement in both interlayer and intralayer interactions during compression, leading to a remarkable modulation of the optoelectronic properties.



IMPACT STATEMENT

By applying pressure, giant enhancement of photocurrent and tunable spectral response range were achieved in NiPS₃, which provides a potential way to modify the optoelectronic properties for materials.

ARTICLE HISTORY

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KEYWORDS

NiPS₃; high pressure; optoelectronic properties; phase transition

1. Introduction

Photodetectors, which generally use semiconductors as absorbing materials and convert optical signals into electric signals, are potential candidates for environmentally friendly energy conversion [1]. Over the past decade, van der Waals materials, such as black phosphorus (BP) [2,3], graphene [4], and transition metal dichalcogenides (TMDCs) [5,6], are widely used in the fabrication of photodetectors [7,8]. However, drawbacks such as weak switching characteristics in graphene, air instability in BP, and narrow wavelength detection range (1.2–2 eV) in TMDCs have limited their further applications in optoelectronic fields [9]. Metal phosphorus trichalcogenides (MPTs) have recently attracted substantial interest [10] because of their wide bandgap range (1.3–3.5 eV) [11]

and stable interlayer structures [12]. Since their discovery in the late nineteenth century [13], MPTs have been widely studied in the electrocatalytic [14], electrochemical [15], and optoelectronic [16] fields. Nickel phosphorus trichalcogenide (NiPS₃), the most representative MPT, has seen a surge of interest [17,18]. NiPS₃ is a charge-transfer insulator [19], and has a thickness-tunable bandgap and air stability [20], indicating its potential in optoelectronic applications. Ultraviolet photodetectors [16] and n-type field-effect transistors (FETs) [21] have been fabricated using NiPS₃, with excellent optoelectronic properties under ambient conditions.

The application of pressure is a controllable approach for tailoring the physical and chemical properties of materials by changing the interatomic distances [22],

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electronic structures [23–25], and crystal structures [26,27]. For example, CrPS₄ has been reported to have a direct-to-indirect bandgap crossover due to pressure-driven lattice rearrangement [28]. Under compression, FePS₃ and FePSe₃ undergo isostructural and quasi-isostructural phase transitions, respectively, and superconductivity has been observed in FePSe₃ with a maximum T_c of 5.5 K via pressure-induced spin-crossover [29]. Similar pressure-induced structural transitions have been observed in MnPS₃ [30], V_{0.9}PS₃ [31], and CoPS₃ [32]. Despite the growing number of studies on MPX₃, the high-pressure behavior of NiPS₃ remains largely unexplored. Low-temperature Raman spectra have shown that NiPS₃ exhibits two-magnon excitation [33] and a strong dependence on the pressure [34], reflecting the pressure-tuning of electronic transitions. An insulator-to-metal transition was studied in a theoretical work [35] and recently proven in pressurized bulk NiPS₃, attributed to interlayer slippage under high pressures [36]. Previous studies on the high-pressure treatment of such materials mainly focused on the correlation between the structural changes and electrical transport properties, ignoring the influence of pressure on the optoelectronic properties. Moreover, although the high-pressure technique is considered a powerful method to regulate the optoelectronic properties of materials [37], obtaining a higher gain and maintaining the excellent high-pressure properties under ambient conditions remain challenging.

In this study, we focused on the optoelectronic properties of NiPS₃ manipulated by the application of pressure. High-pressure in situ photocurrent measurements revealed a significant enhancement in the photoresponse of NiPS₃. The response range could be extended to the near-infrared range under compression. Moreover, the photocurrent of NiPS₃ retained a two-order-of-magnitude increase after pressure release. In situ X-ray powder diffraction (XRD) analysis, Raman measurements, and theoretical calculations demonstrated a significant enhancement in both interlayer and intralayer interactions in NiPS₃, which contribute to its fascinating optoelectronic properties under pressure.

2. Materials and methods

2.1. Sample characterization

Single crystals of NiPS₃ were purchased from Shanghai Onway Technology. The UV-vis absorption data were acquired using an iHR320 spectrometer. Under ambient conditions, Raman spectra excited at 514 nm wavelength were collected by Renishaw. The XRD at 1 atm

is measured by a Rigaku Synergy Custom FR-X diffractometer ($\lambda_{\text{Mo}} = 0.7099 \text{ \AA}$).

2.2. High-pressure measurements

In situ optoelectronic measurements were conducted in diamond anvil cells. The photocurrents and I–V curves were collected using a source meter (Keithley 2461). A 300 W Xe lamp (CEL-HXF300) was used in the first run, while a UVIRCUT400 filter was added in the second run. The illuminated power intensity can be modulated by changing the input current of Xe lamp. A 1650 nm laser was employed for the near-infrared optoelectronic measurements. The high-pressure synchrotron XRD experiments were performed at 4w2 beam line of the Beijing Synchrotron Radiation Facility (BSRF). The MAR345 Charge Coupled Device (CCD) detector (Rayonix) was used, and the vertical $\times$ horizontal focus spot size is $26 \mu\text{m} \times 8 \mu\text{m}$. The sample-to detector distance is 237.0 mm. The wavelength of the X-ray beam was $0.6199 \text{ \AA}$. Silicone oil was placed in a sample chamber to provide a quasi-hydrostatic environment. The obtained XRD patterns were refined using the GSAS software package with the Rietveld methods. Raman spectrum data were acquired using a Renishaw inVia Raman microscope under a 514 nm laser. KBr and c-BN were used as the high-pressure transmitting medium, respectively.

2.3. Theoretical calculations

The ELF of NiPS₃ were calculated using the density functional theory in the generalized gradient approximation employed in the Vienna ab initio simulation package (VASP) code. The projected augmented wave (PAW) method and the Perdew–Burke–Ernzerhof (PBE) exchange correlation were used.

3. Results and discussion

Figure 1(a,b) shows the typical crystal structure of NiPS₃. Within the layer, six Ni atoms form a graphene-type honeycomb lattice, and each $[\text{P}_2\text{S}_6]^{4-}$ unit is located at the center of the honeycomb [38]. Single-atomic layers are connected by weak van der Waals interlayer interactions. As shown in Figure 1(d), NiPS₃ adopts a monoclinic structure with the space group C2/m at ambient pressure [39], and the lattice constants obtained by XRD are $a = 5.788 \text{ \AA}$, $b = 9.991 \text{ \AA}$, and $c = 6.615 \text{ \AA}$. Figure 1(c) shows the Raman spectra of NiPS₃ excited by 514 nm lasers. Consistent with previous reports [40], four in-plane E_g modes and three out-of-plane A_g modes can be observed ($E_g^{(1)}$, 132.3 cm^{-1} , $E_g^{(2)}$, 174.5 cm^{-1} , $A_{1g}^{(1)}$,

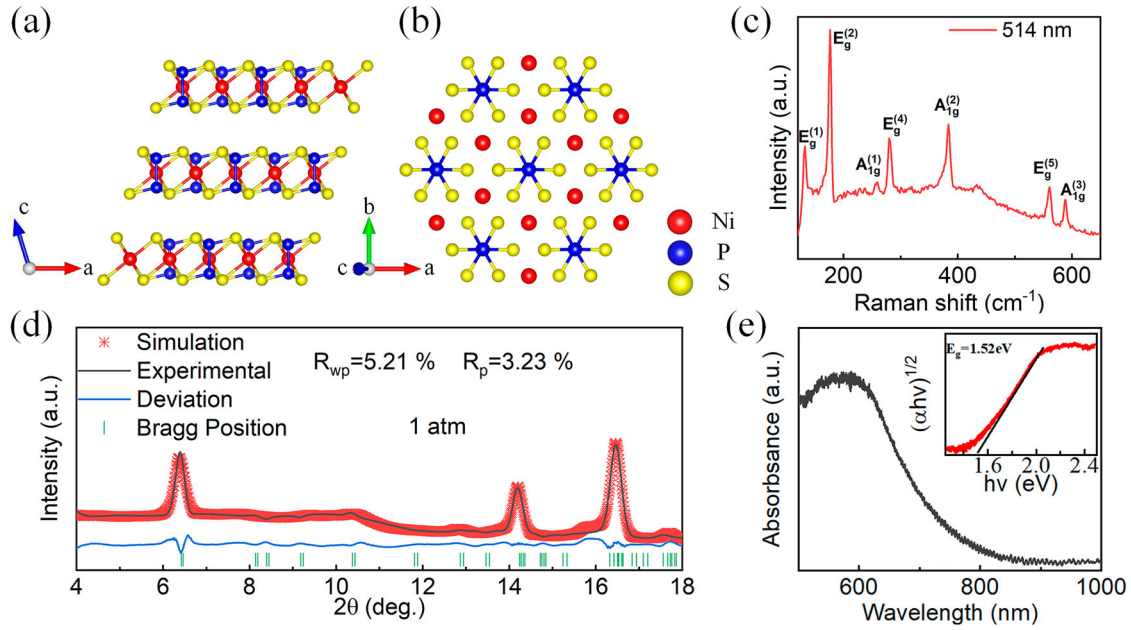


Figure 1. Crystal structure of layered NiPS₃ viewed (a) along the b-axis. (b) top view. (c) Raman spectra of NiPS₃ acquired under ambient conditions. (d) XRD pattern of NiPS₃ with the space group C2/m at 1 atm. (e) Optical absorption spectra and the Tauc plot (inset) of NiPS₃ with a bandgap of 1.52 eV.

257.4 cm⁻¹, $E_g^{(4)}$, 279.6 cm⁻¹, $A_{1g}^{(2)}$, 383.4 cm⁻¹, $E_g^{(5)}$, 560.5 cm⁻¹, $A_{1g}^{(3)}$, 588.5 cm⁻¹). The absence of $E_g^{(3)}$ is probably due to the selective resonance enhancement dominated by electron–phonon coupling. The optical absorption spectrum of NiPS₃ is presented in Figure 1(e). According to the previous report [41], NiPS₃ is an indirect semiconductor. Using the Tauc plot method [42], the band gap E_g is determined to be 1.52 eV, which is similar to a previous result (1.6 eV) [43].

In situ optoelectronic measurements were performed to explore the influence of pressure on the photoresponse of NiPS₃; the setup is shown in Figure 2(a,b). The photoresponse of NiPS₃ at 0.7 GPa was measured under illumination by a Xe lamp at different constant voltages and incident light powers (Figure 2(c)). The photocurrent density J_{ph} and responsivity R are necessary for a detailed analysis of the optoelectronic properties of NiPS₃. The formulae for calculating J_{ph} and R are as follows [44]:

$$J_{ph} = \frac{I_{ph}}{S} \quad (1)$$

$$R = \frac{I_{ph}}{P_{in}S} \quad (2)$$

where I_{ph} is the photocurrent, that is, $I_{ph} = I_{illumination} - I_{dark}$, S is the illuminated active area, and P_{in} is the incident light density. The S and P_{in} values are $1.9 \times 10^{-3} \text{ cm}^2$ and $1.9\text{--}3.5 \text{ mW cm}^{-2}$ for the full-spectrum of the light incident by the Xe lamp, respectively. P_{in} (1.9 mW cm^{-2}) was fixed during the high-pressure

measurements. Figure 2(d) shows J_{ph} and R values of NiPS₃ as a function of the illumination intensity, indicating a good photoresponse performance. Figure 2(e) shows the I–V curves of NiPS₃ under different incident light power densities at 0.7 GPa. The photocurrent gradually increases with an increase in the voltage from -5 to 5 V . The nonlinear characteristics of the output curves indicate the possible existence of a Schottky barrier between NiPS₃ and the Pt electrodes.

Figure 3 shows the photocurrents of NiPS₃ during compression and decompression cycles under illumination by a Xe lamp at a voltage of 1 V . The obviously increased recovery time in Figure 3(a, b) is caused by the photothermal effect. Figure 3(c) shows the extracted J_{ph} and R values as a function of the pressure; Figure S1b shows the resistance. With increasing pressure, J_{ph} (R) of the sample shows a gradual increase up to 5.7 GPa , followed by a rapid increase up to 14.1 GPa . After that, the photoresponse vanishes upon further compression because of the pressure induced insulator–metal transition in NiPS₃. The R value at 5.7 GPa reaches up to approximately $6.8 \times 10^{-3} \text{ A W}^{-1}$ ($J_{ph} = 1.1 \times 10^{-2} \text{ mA cm}^{-2}$), which is an order of magnitude higher than 0.7 GPa ($R = 1.9 \times 10^{-4} \text{ A W}^{-1}$, $J_{ph} = 3.1 \times 10^{-4} \text{ mA cm}^{-2}$). Further compression increases the responsivity more rapidly, reaching as high as 24.0 A W^{-1} ($J_{ph} = 38.9 \text{ mA cm}^{-2}$) at 14.1 GPa . The R and J_{ph} values at this pressure were enhanced by approximately five orders of magnitude over their initial values at 0.7 GPa . Remarkably, as shown in Figure 3(c),

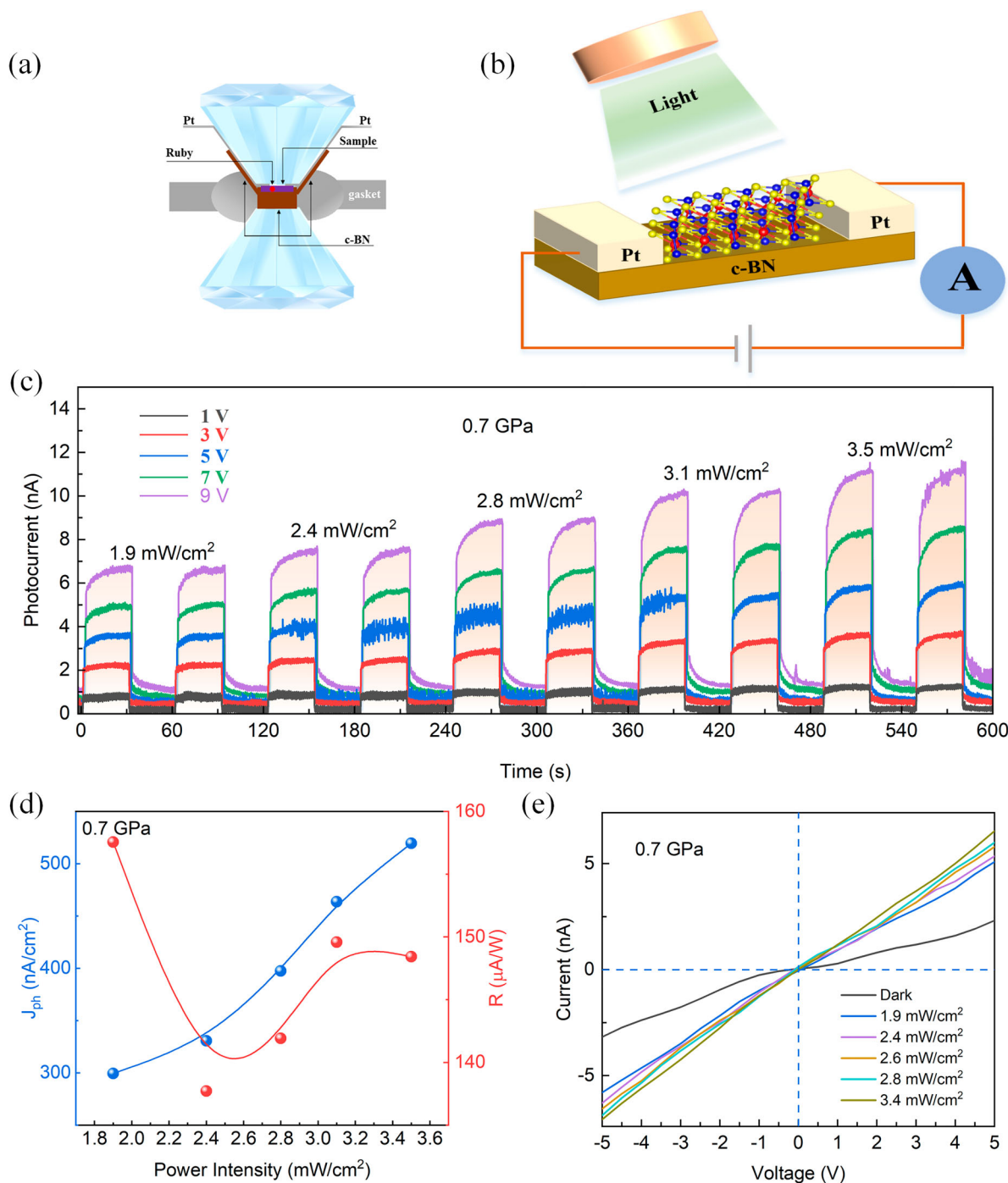


Figure 2. (a) Schematic of high-pressure DAC setup. (b) in situ photoelectronic measurements for NiPS₃ device. (c) Photocurrents of NiPS₃ varying with different voltages and incident light power intensities at an applied pressure of 0.7 GPa. (d) J_{ph} (blue) and R (red) versus the light power intensity at a voltage of 1 V. (e) I–V curves of NiPS₃ under different light power intensities at 0.7 GPa. Xe lamp serves as source of illumination.

when decompression was performed to the lowest pressure (1 atm), the photocurrent is 138.2 nA and the values of R and J_{ph} were still two orders of magnitude higher than those at the initial pressure of 0.7 GPa during compression. The decompressed sample was then left for several days to investigate the stability of its optoelectronic properties. As shown in Figure S2, the

photocurrent of NiPS₃ decreases quickly in the first 24 h and then stabilizes gradually. After 120 h, the photocurrent remains almost unchanged at 20.2 nA, which is still a 34-fold retention compared with the initial value (0.7 GPa, 0.58 nA). Furthermore, the illuminating range was narrowed down to the visible light region in the second experiment cycle (Figures S3 and S4). The results

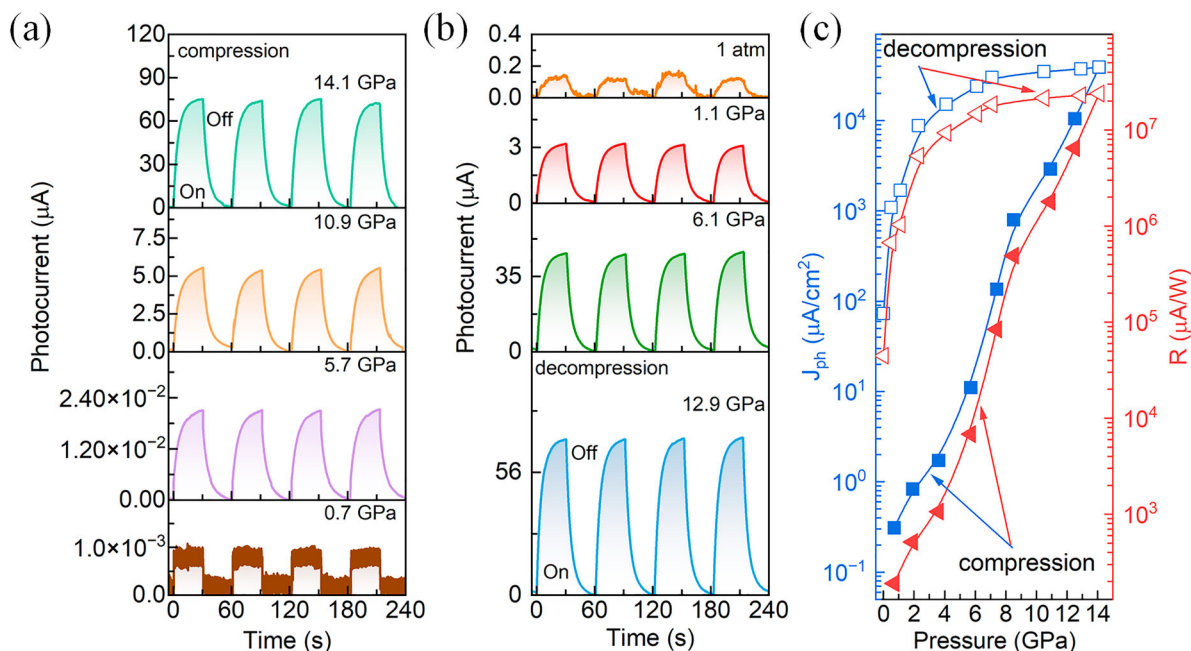


Figure 3. NiPS₃ photocurrent during (a) compression and (b) decompression under illumination by Xe lamp at 1 V. (c) Pressure-dependent J_{ph} and R during compression and decompression extracted from (a) and (b).

show that the pressure-induced enhancement in the photocurrent in NiPS₃ is highly repeatable. Pressure-driven irreversible properties of several materials have been reported. For example, in PbBiO₂Br, although the structural and optical properties are partially retained after decompression, the optoelectronic response is strongly reversed [45]. After two compression-cycle treatments, perovskite CH₃NH₃SnI₃ [46] shows higher photocurrents at 0.7 GPa than the initial values; whether the properties could be stabilized after release remains unclear. Eu³⁺-doped CsPbCl₃ quantum dots [44] showed a two-fold increase in the photocurrent after pressure release. To the best of our knowledge, our study is the first to achieve such a significant enhancement in the photocurrent after decompression to ambient pressure, with excellent stability even after 120 h. As shown in Figure 1(e), NiPS₃ is an indirect semiconductor with a bandgap of 1.52 eV. Thus, the absorption threshold of NiPS₃ is 815 nm under ambient conditions. To investigate the effect of pressure on the spectral response region of NiPS₃, we measured the high-pressure photocurrents under 1650 nm laser illumination at a voltage of 5 V. As shown in Figure S1a, when the pressure increases to 6.1 GPa, NiPS₃ starts to absorb light photons incident at 1650 nm and shows a positive correlation between the photocurrent and pressure. This indicates that the spectral response region of NiPS₃ can be regulated by longer-wavelength NIR light.

Figure 4 shows the XRD patterns for pressures of up to 50 GPa and the evolution of the d-spacings under

pressure. Upon compression, the intensity of the peak $\sim 14.5^\circ$ decreases with increasing pressure and finally disappears above 15.0 GPa. Meanwhile, a new diffraction peak emerges at 15.0 GPa, indicating a new phase (phase II). With continuous compression to 31.4 GPa, the peak at $\sim 6^\circ$ vanishes, and another new peak suddenly appears at $\sim 15.7^\circ$, whose intensity is positively correlated with the pressure. The observed phenomena suggest a transition from phase II to the second high-pressure phase (phase III).

According to previous research [36], an isostructural transition from phase I to phase II is manifested by the sudden changes in lattice parameters. The lattice parameters a , b , and c decrease with increasing pressure in the pressure range of 0–15 GPa, with the compressibility being particularly high along the c -axis. In addition, there appears to be a change in the slope for all the unit cell parameters at approximately 5.8 GPa. In the pressure range of 5.8–15 GPa, the variations in the three parameters with pressure are reduced. This change can be attributed to the transition interval [36].

Figure 5(a) shows the selected Raman spectra of NiPS₃ measured at pressures ranging from 0.5–22.5 GPa. By analyzing the Raman spectra, several changes can be observed in the transition interval region. We observed the emergence of the Raman mode $E_g^{(3)}$ at 7.7 GPa. The high-pressure XRD results show that the lattice parameters vary under the application of pressure, resulting in a variation in the Raman tensor [36]. Consequently, the Raman mode $E_g^{(3)}$ occurs under a pressure of 7.7 GPa.

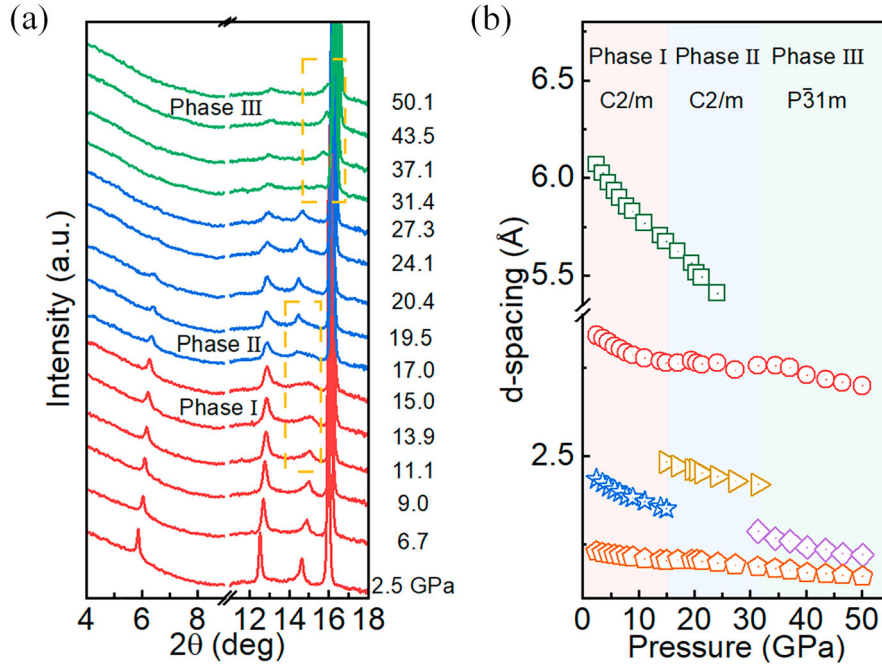


Figure 4. (a) High-pressure XRD patterns of NiPS_3 in compression. (b) Evolution of d-spacing with increasing pressure.

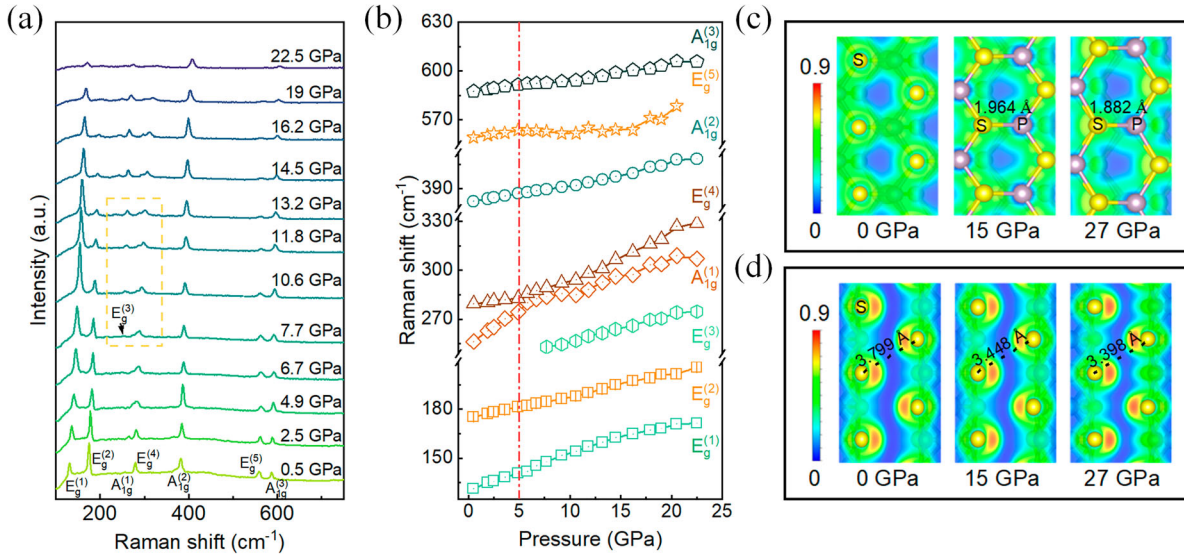


Figure 5. High-pressure Raman spectra of NiPS_3 : (a) Selected Raman spectra at various pressures. (b) Pressure dependence of Raman shifts. (c) Electron localization function (ELF) of intralayers in NiPS_3 . (d) ELF of interlayers in NiPS_3 .

During compression (Figure 5(b)), most of the Raman modes shift toward higher frequencies, except for $E_g^{(5)}$. The $A_{1g}^{(1)}$ and $E_g^{(4)}$ modes merge into a single mode at 5 GPa, whereas they split again at 10.6 GPa. According to a previous report [40], the $E_g^{(4)}$ mode contains both in-plane vibrations of the Ni atoms and $[P_2S_6]$ units, while the $A_{1g}^{(1)}$ mode is closely related to the van der Waals interaction. Upon compression, the rapid movement of the out-of-plane vibration mode $A_{1g}^{(1)}$ below 4.9 GPa demonstrates that the interlayer interaction is

significantly enhanced. Above 4.9 GPa, the condition is reversed. The in-plane mode $E_g^{(4)}$ moves faster with the pressure than the $A_{1g}^{(1)}$ mode, and finally, peak splitting occurs at 10.6 GPa. The $E_g^{(5)}$ mode contains the strongest horizontal-vibration components of the P–P dimers, while the Ni atoms are at rest. A redshift in the $E_g^{(5)}$ mode is observed in the transition interval.

Finally, the mechanism underlying the pressure-enhanced optoelectronic properties of NiPS_3 was investigated. According to previous research [36], the rapid

decrease in all the values along the three axes indicates that the pressure can effectively modulate the interlayer and intralayer interactions of NiPS₃. Enhanced atomic interactions could also be confirmed from the Raman spectroscopy measurements. In the pressure range of 0–4.9 GPa, the fusion of $A_{1g}^{(1)}$ and $E_g^{(4)}$ Raman peaks suggests an enhancement in the interlayer interaction. Following the transition interval, the $A_{1g}^{(1)}$ mode exhibited a nonlinear correlation with the pressure and finally split from the $E_g^{(4)}$ mode at 10.6 GPa. The rapid shift in $E_g^{(4)}$ demonstrates that further compression has a more effective influence on the intralayer than on the interlayer at higher pressures. Notably, previous theoretical calculations [36] indicate the formation of covalent-like bonds between the S and P atoms in adjacent layers in the phase II structure. In our study, the dramatically reduced interlayer spacing below 4.9 GPa is comprehensible because of the weak van der Waals interlayer interactions. Above 4.9 GPa, the new chemical bonds formed between the [P₂S₆] units from different layers make the in-plane Raman mode $E_g^{(4)}$ to respond more intensively to the pressure. The decreasing rate of the $A_{1g}^{(1)}$ mode indicates that the newly formed S–P bonds between the layers have a lower contraction ratio than before, which is similar to that observed in ReS₂ [5]. This conclusion is consistent with the XRD results, where changes in the slope are observed in the transition interval. In addition, the redshift of the $E_g^{(5)}$ mode in the pressure range of 5–12 GPa can be understood as phonon softening, which has been observed in other materials [47]. Phonon softening typically signifies rapid charge transfer. Previous studies [48] have demonstrated the p-type behavior of pure NiPS₃. For a p-type semiconductor, the formula $\sigma = \mu \times p$ (where σ is the conductivity, μ is the mobility ratio, and p is the hole concentration) plays an important role in the optoelectronic process [49]. In NiPS₃, pressure-induced shortened distances enhance both the intralayer and interlayer interactions, leading to an increase in the charge transfer mobility. Hence, the increased μ under pressure causes a high conductivity, which eventually contributes to photocurrent enhancement.

To further understand the effect of pressure on the charge transfer in NiPS₃, the electron localization function (ELF) was calculated at selected pressures. As shown in Figure 5(c and d), both the S–S interlayer distances and S–P intralayer distances are reduced under compression. Under the application of pressure, electron charge transfer occurs not only from S to S but also from S to P. Both the enhanced interlayer and intralayer interactions explain the efficient pressure modulation of the optoelectronic properties of NiPS₃.

Furthermore, we investigated the possible reason for the pressure-induced retainability of the photocurrent. The Raman spectra of NiPS₃ kept for different durations after decompression to ambient conditions are shown in Figure S2b. Compared with the original NiPS₃, the decompressed sample exhibited a significant blueshift in all the Raman modes, indicating local bonding changes in the sample. The distinction between the Raman peaks shows that NiPS₃ maintains a high residual strain after decompression [50]. Unlike most previously reported materials exhibiting decompression-reversible optoelectronic properties, the durable strain in NiPS₃ maintains excellent high-pressure properties after decompression.

4. Conclusions

In summary, a significant pressure-induced photocurrent enhancement was observed in NiPS₃. Upon compression, the maximum photocurrent in NiPS₃ was five orders of magnitude higher than the initial value. The partial photocurrents were retained after decompression. Additionally, the photoresponse range of NiPS₃ was successfully extended to the infrared range by applying pressure. Based on XRD, Raman spectra, and theoretical calculations, we conclude that, during the phase transition, the reduced atomic distance and chemical bonds newly formed under pressure significantly enhanced the interlayer and intralayer interactions, resulting in remarkable pressure-enhanced optoelectronic properties of NiPS₃. The successful realization of the pressure-tuned optoelectronic properties of NiPS₃ is expected to provide new ideas for the modification of other materials.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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