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Examining NiPS3: Properties, Application, and Challenges

Jake Huang

Polytechnic School, Pasadena, CA, USA
Email: jhuang25@students.polytechnic.org

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Abstract

The unique structural and electrical properties of two-dimensional van der Waals (vdW) material, nickel-phosphorus trisulfide ($NiPS_3$), render it a promising compound for its adaptation in advanced technology applications. In order to explore its potential practical applications in optoelectronic, spintronic, and energy conversion technologies, this work has explored some of the fundamental aspects defining the excitonic behavior of $NiPS_3$, such as bandgap characteristics, antiferromagnetism, and semiconductor nature derived from its layered structure. This study of the properties of $NiPS_3$ would also outline problems or difficulties that must be faced upon its use in new technologies. This also indicates the demand for further research on $NiPS_3$ to fulfill or realize its promise in technological advancement more fully.

Keywords

$NiPS_3$, 2D Materials, Van der Waals Materials, Bandgap Engineering, Semiconductors, Spintronics, and Materials Science

1. Introduction

Two-dimensional (2D) materials have transformed materials science due to their unique physical and electrical characteristics resulting from their atomic-scale thickness and strong in-plane bonding [1] [2]. Van der Waals materials, such as $NiPS_3$, have weak interlayer forces and may be mechanically exfoliated into single or few-layer structures. This property allows for novel quantum phenomena, such as increased exciton binding energies, which are substantially more prominent in 2D systems than in bulk materials due to lower dielectric screening and quantum confinement effects.

Band theory is a prominent theory in materials science that explains how certain physical properties in solid materials manifest through interactions between the conduction band and valence band in materials. Electrons in the conduction band can move and conduct electricity, while electrons in the valence band may jump into the conduction band [3]. The bandgap, or the energy difference between the conduction band and the valence band, determines electrical conductivity: band overlap indicates materials with high conductivity while massive bandgap indicates insulating properties [4], as seen in **Figure 1**. Semiconducting materials have bands with lesser band gaps, allowing electrons to jump from the valence band to the conduction band through energy input [5].

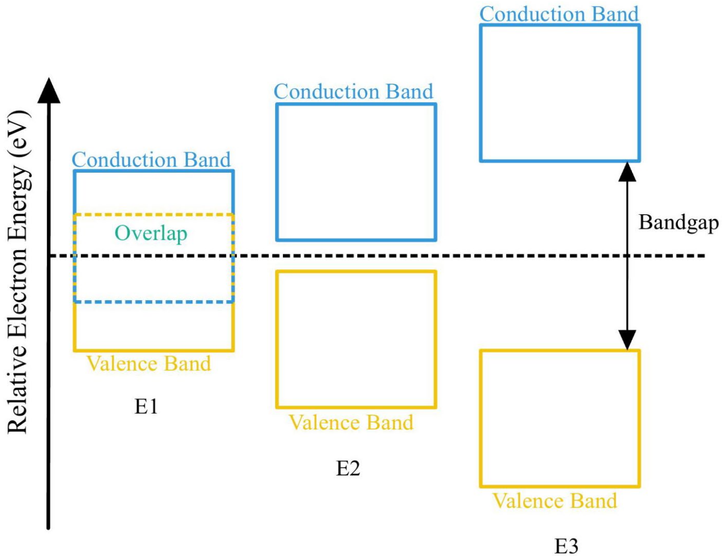

Figure 1. Bangap in metals. E1-onductor, E2-emiconductor, E3-nsulator. Metals with overlapping conduction and valence bands like in E1 do not need to overcome some energy barrier in order to move electrons from the valence to the conduction band, so they have high electrical conductivity. Both insulators (E3) and semiconductors (E2) have a bandgap, but bandgaps are surmountable, allowing the semiconductor to conduct electricity.

In 2D materials, strain, electric fields, and chemical doping can be used to tune the bandgap, allowing for increased versatility in photonic and electronic device engineering [6]. Excitons are an especially large area of focus when it comes to optoelectronic properties of 2D materials. They are a type of quasiparticle that appears from the electromagnetic binding of electrons and holes and can be observed just under the bandgap in energy graphs. Excitons are prevalent among materials with direct bandgaps, and due to their dominance in light-matter interactions, materials with exciton interactions are suitable for photodetectors and light-emitting diodes (LEDs) [7].

Néel temperature is also an important factor to consider when looking at antiferromagnetic materials like $NiPS_3$. Below the Néel temperature, magnetic moments align antiparallel to each other or, in other words, become antiferromagnetic. This magnetic feature is important when researching spintronic applications as spintronics process information through electron spin rather than through electron charge like in electronics [8].

2. Properties and Structure of $NiPS_3$

$NiPS_3$ belongs to the class of transition metal thiophosphates. It crystallizes in a layered structure with each layer made up of nickel atoms coordinated by sulfur and phosphorus atoms and is suitable for mechanical exfoliation to the monolayer limit because of the weak van der Waals forces holding its layers together [2]. For this material, the direct bandgap allows for direct application in optoelectronic devices requiring effective light absorption and emission. $NiPS_3$ has a tunable bandgap that can be changed by external factors like strain, therefore making it suitable for a wide range of applications [6]. Compared to that of MoS_2 and other transition metal dichalcogenides, the layered structure of $NiPS_3$ brings out strong in-plane electronic coupling, which contributes to higher charge mobility in the monolayer form [5]. The bandgap value for $NiPS_3$ was measured at 1.5 eV, positioning this material as an ideal candidate for optoelectronic devices [7].

To date, $NiPS_3$ crystals synthesized have relied greatly on chemical vapor transport (CVT) in their methodology, a process with iodine as the transport agent to deposit $NiPS_3$ crystals using a temperature gradient [9]. This approach yields crystal sizes of about 1 cm^2. Mechanical exfoliation can still be employed as a practical method to study this material on a very small-scale basis. Methods like X-ray diffraction (XRD) and Raman spectroscopy confirm the quality of crystallinity and layer dependence in the bandgap [10].

Antiferromagnetic order arises in $NiPS_3$ below a Néel temperature of about 150 K, where nickel atoms exhibit antiparallel magnetic moments [8] [11]. The complex magnetic ordering below the Néel temperature was unraveled by carrying out Mössbauer spectroscopy and neutron diffraction experiments. In fact, these studies have evidenced the presence of a zigzag antiferromagnetic structure that makes $NiPS_3$ a potential candidate in the low-temperature application of a spintronic device [10]. $NiPS_3$ also exhibits anisotropic conductivity, with higher in-plane conductivity compared with out-of-plane directions. In-plane conductivity reaches a value over 10^3 S/m, which is much larger than the conductance in out-of-plane directions. This property is important in the construction of electronic devices that require high directional conductance, such as field-effect transistors [9].

3. Applications of $NiPS_3$

The direct bandgap and strong excitonic effects make $NiPS_3$ a highly desirable candidate for applications in the domain of optoelectronics. For example, $NiPS_3$ can improve efficiency and other aspects of LEDs, photodetectors, and light-sensitive devices. The property of externally tuning its band gap also improves its use cases in devices that need specific wavelength responses. Importantly, $NiPS_3$ has already proven itself to be competitive with conventional materials when it comes to field-effect transistors (FETs), which controls electrical behavior in devices using an electric field. It has shown an on/off ratio of around 10^3 - 10^5 at 25˚C and threshold voltages of 0.5 - 1.5 V when using bulk and few-layer $NiPS_3$ [10].

$NiPS_3$ has huge promise in the field of photodetection. While the responsivity rates for traditional MoS_2-based devices normally stands at around 100 - 150 A/W, responsivity rates in $NiPS_3$-based photodetectors reached above 200 A/W, a sizable increase [10]. Such high responsivity allows $NiPS_3$ to outperform many traditional materials used in different optoelectronic applications and make appropriate adjustments of the bandgap feasible. In terms of mobility, the mobility value of the advanced $NiPS_3$-based FETs lie in the range of 0.5 - 1 cm^2/Vs. Although this is a little less than some other high-mobility materials, optimizations can be made using top-gated structures or high-k dielectric materials. Compared to graphene, which lacks a natural bandgap, $NiPS_3$'s intrinsic semiconducting nature also offers more control over electronic properties, making it more suitable for specific applications like transistors [5].

Recent studies have shown that $NiPS_3$ performs very well in hydrogen evolution reactions (HER) and oxygen evolution reactions (OER), crucial aspects of water-splitting processes. For example, $NiPS_3$ in HER exhibited an overpotential of 158 mV at 10 mA/cm^2, far superior to Pt-based catalysts [10]. Regarding $NiPS_3$ in OER, it only needed an overpotential as low as 300 mV at a current density of 10 mA/cm^2, outperforming standard RuO_2-based catalysts, which require higher overpotentials. Because it possesses bifunctionality, $NiPS_3$ can play a dual role not only as an anode but also as a cathode in water electrolyzers and hence becomes an ideal candidate for application in sustainable energy devices with particular relevance to high-efficiency water-splitting technology developments. The stability of $NiPS_3$ during these reactions could maintain more than 95% of its activity for 24 hours, further underlining its usability in long-term energy conversion systems.

With a tunable bandgap and layered structure, $NiPS_3$ is a strong potential application in next-generation flexible electronic devices. It has already been demonstrated that flexible photodetectors using $NiPS_3$ ensure a 30% gain in photodetection efficiency with respect to devices using MoS_2 upon testing with near-infrared light [12]. High electronic performance places $NiPS_3$ as a highly important material toward upcoming flexible electronics, such as foldable displays, wearable sensors, and other variable deformation optoelectronic devices [5] [10].

Finally, recent studies in $NiPS_3$ point towards potential for memory storage and spintronics. Below 150 K, antiferromagnetic ordering in $NiPS_3$ allows it to be applied in low-temperature devices of spintronics, where information is stored and treated by electron spin rather than charge carriers, a property opposite to traditional electronics. It expands possible applications in magnetic memory storage and energy-efficient logic circuits that are alternatives to conventional electronics [13] [14].

4. Challenges

Despite the slew of promising qualities of $NiPS_3$, a number of challenges remain to hinder large-scale implementation. First, the large-scale synthesis of high-quality $NiPS_3$ crystals is a significant barrier. Current chemical vapor deposition (CVD) methods have resulted only in up to 1 cm^2 crystals–insufficient for large-scale applications [9]. Optimizations are currently being done in CVD mainly through reaction temperature and precursor concentration. Separate from CVD, promising results in industrial-scale production have been obtained through an electrochemical cathodic exfoliation technique. With this technique, a negative voltage is applied to bulk $NiPS_3$ crystals in an electrolyte solution, which causes large tetra-n-butylammonium ions to intercalate between $NiPS_3$ layers, weakening van der Waals forces. The ions decompose into gas to create pressure and separate the layers, resulting in the production of high-quality $NiPS_3$ flakes. Using this method, $NiPS_3$ flakes as large as 150 μm^2 have been successfully produced with yields of up to 80%, surpassing traditional liquid-phase exfoliation techniques, which struggle to produce such large flakes consistently [15]. Sonication, using ultrasonic waves to overcome van der Waals forces between layers, is sometimes used in other exfoliation methods. Electrochemical cathodic exfoliation is a sonication-free process, further eliminating the potential structural damage that is often seen in other methods and maintaining the high-quality crystal integrity of $NiPS_3$. Other approaches that require sonication, like liquid-phase exfoliation, yield flakes of $NiPS_3$ in much higher concentrations, such as 10 mg/mL [5].

The electrochemical exfoliation technique also provided fast production. CVT and liquid-phase exfoliation methods usually take hours or even days to mass-produce the desired crystals. With electrochemical exfoliation, the process becomes mere minutes. This method is fairly efficient in the large-scale production of high-quality, atomically thin $NiPS_3$ crystals, with a high monolayer ratio of about 70%. Further optimization, through voltage bias or the type of intercalation agents, can lead to higher yield and better structural quality [15].

Another issue that $NiPS_3$ faces is its low Néel temperature of 150 K, limiting its integration at room temperature into spintronic devices. Attempts at doping using elements such as manganese or iron have come up with as much as 20 K rises in the Néel temperature, but further studies are needed to push this boundary much further without sacrificing other desirable properties. These improvements in the Néel temperature, though small, indicate that there could be future breakthroughs via material engineering and alloying methods [10].

Finally, environmental stability is a present concern because $NiPS_3$ decomposes under exposure to moisture and oxygen [16]. Many studies with environmental testing demonstrate that $NiPS_3$ degrades within 48 hours of exposure to ambient conditions. Protective coatings such as hexagonal boron nitride (h-BN) have been shown to extend $NiPS_3$'s stability to over a week in ambient air, although further optimization is needed to maintain performance while minimizing the loss of the material's intrinsic properties. Research on multilayer encapsulation techniques and inert atmosphere storage solutions may also present viable pathways to mitigate environmental degradation for large-scale, practical use.

5. Discussion

While this study provides valuable insights into $NiPS_3$, some methodological issues warrant attention. Many experiments were conducted under controlled conditions that may not reflect real-world applications, particularly in studies on magnetic properties and Néel temperature [17]. Additionally, the small sample sizes due to the difficulty in synthesizing high-quality $NiPS_3$ crystals introduce variability and raise concerns about the generalizability of the results [12]. Addressing these issues in future research could enhance the reliability and applicability of the findings, thereby strengthening the understanding and utility of $NiPS_3$ in practical applications.

6. Conclusions

Because of its tunable bandgap, excitonic behavior, antiferromagnetism, and anisotropic conductivity, $NiPS_3$ is a very promising candidate for optoelectronics, spintronics, and energy conversion applications.

Still, numerous challenges stop $NiPS_3$ from fully realizing its potential. First, despite recent doping strategies to increase the material's Néel temperature, its low Néel temperature at 150 K makes use in room-temperature spintronics and other devices very challenging, if not impossible. The increases in Néel temperature are also extremely incremental (a maximum of 20 K) [8] [12]. In addition, current methods in industrial-scale synthesis are difficult, time-consuming, and inefficient. Low environmental stability further stifles the implementation in current technology. Further research should attempt to circumvent or offer a solution to $NiPS_3$'s various challenges. The properties of $NiPS_3$, put into perspective by continuous advances in its research, establish a place within the broader context of 2D materials and their applications.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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