

# Exploring Tunable Properties of Tellurene van der Waals Heterostructures for Nanoelectronic Applications

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## Abstract

Two-dimensional (2D) tellurium, known as tellurene, has emerged as a promising post-graphene material due to its unique electronic, optical, and structural properties. Its intrinsic in-plane anisotropy, strong spin-orbit coupling, thickness-dependent tunable bandgap, and excellent environmental stability make it highly suitable for nanoelectronic and optoelectronic applications. The construction of van der Waals (vdW) heterostructures by integrating tellurene with other 2D materials such as transition-metal dichalcogenides offers additional degrees of freedom for tailoring material properties through interlayer coupling, strain engineering, stacking configuration, and external electric fields. This review systematically examines recent advances in tellurene-based vdW heterostructures, emphasizing tunable electronic and optical properties, band alignment engineering, and device-level performance. Key challenges and future research directions toward scalable nanoelectronic applications are also discussed.

*Keywords:* Tellurene; van der Waals heterostructures; two-dimensional materials; bandgap engineering; nanoelectronics

## Introduction

In recent years, two-dimensional (2D) elemental tellurium, also known as tellurene, has emerged as a promising post-graphene material for next-generation nanoelectronics and optoelectronics. First predicted theoretically and subsequently synthesized experimentally, tellurene exhibits multiple stable monolayer allotropes ( $\alpha$ -,  $\beta$ -, and  $\gamma$ -phases) with distinct

lattice configurations and electronic characteristics (Kang et al., 2018). Its quasi-one-dimensional helical chain structure results in pronounced in-plane anisotropy, enabling direction-dependent carrier transport, strong spin–orbit coupling, and a tunable bandgap ranging from approximately 0.35 to 1.2 eV depending on thickness and strain. These features, combined with excellent environmental stability and high carrier mobility, position tellurene as an attractive candidate for field-effect transistors (FETs), photodetectors, thermoelectric generators, and flexible electronics (Qiao et al., 2018).

The integration of tellurene into van der Waals (vdW) heterostructures further broadens its potential. vdW stacking allows materials with mismatched lattices to be combined without chemical bonding, enabling diverse electronic and optical tunability. When tellurene is paired with transition-metal dichalcogenides (TMDs) such as MoS<sub>2</sub>, WS<sub>2</sub>, or MoSe<sub>2</sub>, or with other 2D semiconductors, the resulting heterostructures exhibit type-I, type-II, or type-III band alignments depending on the interface chemistry and layer orientation (Li et al., 2022). This offers new opportunities for bandgap engineering, charge transfer modulation, and interfacial exciton control, essential for designing multifunctional nanoscale devices.

Recent studies have reported MoS<sub>2</sub>/tellurene and WS<sub>2</sub>/tellurene heterojunctions exhibiting high photoresponsivity and tunable charge transport under strain, gate bias, and electric fields. Trilayer stacks like MoS<sub>2</sub>/ $\alpha$ -Te/WS<sub>2</sub> reveal stacking-dependent modulation of carrier effective mass and interlayer coupling, demonstrating that stacking order, interlayer spacing, strain, and rotational alignment serve as tunable parameters for property control (Liang et al., 2023). Consequently, tellurene-based vdW heterostructures are increasingly recognized as a tunable 2D platform for both fundamental studies and nanoelectronic applications.

This review consolidates current progress on the tunable properties of tellurene vdW heterostructures, focusing on structure–property relationships, external tuning mechanisms, and device applications. It also highlights existing challenges and future directions for realizing scalable tellurene-based nanoelectronic systems.

## 2. Structural and Electronic Properties of Tellurene

Tellurene consists of spiral helical chains arranged in parallel planes connected by weak van der Waals interactions. The  $\alpha$ -phase (monoclinic) is the most thermodynamically stable, while the  $\beta$ - and  $\gamma$ -phases offer distinct lattice symmetries and electronic dispersions (Zhang

et al., 2020). The intrinsic bandgap of monolayer tellurene ( $\sim 1.0$  eV) decreases with increasing layer thickness, approaching bulk tellurium's semiconducting gap ( $\sim 0.35$  eV). This layer-dependent tunability makes it suitable for transistor and photonic applications across infrared and visible ranges.

The material's strong spin-orbit coupling (SOC) and low symmetry produce anisotropic effective masses and direction-dependent mobility, with predicted hole mobilities exceeding  $10^3$  cm<sup>2</sup>/V·s (Li & Zhu, 2021). Moreover, tellurene's inherent environmental stability distinguishes it from air-sensitive 2D materials like phosphorene, ensuring longer operational lifetimes for practical devices.

### **3. Van der Waals Heterostructures and Interfacial Engineering**

vdW heterostructures based on tellurene leverage its high carrier mobility and tunable bandgap to enhance device performance. The weak interlayer forces facilitate stacking with materials of varying band structures to achieve specific band offsets and charge transfer characteristics (Gong et al., 2021).

Computational and experimental studies have demonstrated that combining tellurene with TMDs forms type-II heterojunctions, which are ideal for separating photogenerated carriers across the interface. This property enhances photocurrent and quantum efficiency in photodetectors (Tang et al., 2022). Conversely, type-I alignment configurations are beneficial for light-emitting devices, where electrons and holes recombine in the same layer.

The interface characteristics—including interlayer spacing, twist angle, and defect density—strongly influence charge transport. Advances in deterministic transfer techniques and interface passivation have significantly improved reproducibility and minimized charge traps, leading to more stable and predictable heterostructure behavior (Shi et al., 2023).

## **4. Tunable Physical Properties in Tellurene Heterostructures**

### **4.1 Strain Engineering**

Strain is a powerful means of tuning the bandgap, effective mass, and carrier mobility in 2D materials. In tellurene heterostructures, biaxial tensile strain typically reduces the bandgap and can induce semiconductor-metal transitions (Zhang et al., 2022). The anisotropic lattice

allows direction-dependent strain effects—for example, strain along the armchair direction has a stronger influence on the conduction band minimum compared to the zigzag direction. In heterostructures like MoS<sub>2</sub>/α-Te, applying moderate strain ( $\leq 4\%$ ) can switch the band alignment from type-II to type-I, enabling dynamic control over carrier confinement and exciton behavior (Chen et al., 2021).

#### **4.2 Electric Field and Gate Modulation**

The application of an external perpendicular electric field significantly alters interlayer coupling and charge transfer. In tellurene/TMD heterostructures, gate-induced electric fields can tune the band offsets and potential barriers, resulting in controllable transitions between p–n, n–n, and p–p junction behaviors. Dual-gated FETs based on MoS<sub>2</sub>/tellurene exhibit reversible modulation of photoresponse and on/off current ratio, suggesting strong field-tunable band realignment (He et al., 2022).

#### **4.3 Doping and Chemical Functionalization**

Controlled doping offers another approach to tailor the Fermi level and conductivity of tellurene. Halogen (Cl, Br) or alkali (Na, K) doping modifies carrier concentration while preserving structural stability. Surface adsorption of molecules such as NO<sub>2</sub> or NH<sub>3</sub> on tellurene heterostructures further alters local charge density, enabling gas-sensing and photo-switching functionalities (Huang et al., 2021).

#### **4.4 Twistrionic Effects**

Interlayer rotation or “twist” between tellurene and other 2D layers produces moiré superlattices, modifying interlayer hybridization. Theoretical studies predict that small twist angles ( $< 3^\circ$ ) generate flat electronic bands, enhancing excitonic confinement and potentially enabling correlated quantum phases. Such twistrionic tellurene heterostructures could serve as a novel platform for exploring quantum transport and moiré exciton physics (Guo et al., 2023).

### **5. Device Applications**

#### **5.1 Field-Effect Transistors (FETs)**

Tellurene-based FETs demonstrate high on/off ratios ( $> 10^5$ ) and excellent stability compared to other group-VI 2D materials. Integration with MoS<sub>2</sub> or WS<sub>2</sub> in vdW heterostructures

allows for gate-tunable Schottky barriers and reduced contact resistance. Heterostructure FETs exhibit high mobility (up to  $700 \text{ cm}^2/\text{V}\cdot\text{s}$ ) and low subthreshold swing, making them suitable for low-power logic and flexible circuits (Li et al., 2020).

## 5.2 Photodetectors and Optoelectronic Devices

Type-II band alignment in  $\text{MoS}_2/\text{tellurene}$  and  $\text{WS}_2/\text{tellurene}$  promotes spatial separation of photoexcited carriers, enhancing photoresponsivity ( $>500 \text{ A/W}$ ) and detectivity. The tunable bandgap enables detection across the visible to near-infrared spectrum, while strong spin-orbit coupling allows polarization-sensitive photodetection. These characteristics position tellurene heterostructures as candidates for broadband, high-speed, and polarization-sensitive photodetectors (Wu et al., 2021).

## 5.3 Thermoelectric and Energy-Harvesting Devices

Tellurene possesses low lattice thermal conductivity and a large Seebeck coefficient, favorable for thermoelectric conversion. When coupled with metallic or semiconducting 2D layers (graphene,  $\text{MoS}_2$ ), heterostructured thermoelectric junctions display enhanced power factors and suppressed phonon transport. Simulations predict  $ZT > 1.5$  for optimized multilayer tellurene-based stacks (Sun et al., 2022).

## 5.4 Flexible and Wearable Electronics

The inherent flexibility and air stability of tellurene allow fabrication of bendable heterostructure devices. Tellurene-on-polymer FETs retain  $>90\%$  of mobility after 1000 bending cycles, while tellurene/graphene composites show stable photoresponse under repeated deformation. These characteristics make tellurene vdW heterostructures suitable for wearable optoelectronics and strain sensors (Zhao et al., 2022).

## 6. Challenges and Future Outlook

1. Despite significant progress, several challenges limit the full exploitation of tellurene heterostructures:
2. Interface Quality and Stability: Interfacial contamination, oxidation, and lattice mismatch degrade carrier transport. Clean transfer and encapsulation methods (e.g., h-BN capping) are needed.

3. Scalable Synthesis: Large-area, uniform, monolayer tellurene growth remains difficult. Advanced CVD or MBE processes with in-situ monitoring could address reproducibility issues.
4. Contact Engineering: High contact resistance and Schottky barriers reduce device efficiency; work-function-matched electrodes and tunneling layers may mitigate these issues.
5. Integration with CMOS Platforms: Compatibility with silicon-based processes is essential for commercialization; hybrid fabrication routes must be explored.

## Conclusion

Tellurene-based van der Waals heterostructures represent a versatile and highly tunable platform for next-generation nanoelectronic and optoelectronic devices. The combination of tellurene's intrinsic anisotropic transport, tunable bandgap, and strong spin-orbit coupling with the flexibility of vdW stacking enables precise control over interfacial electronic structures and charge transport mechanisms. Recent theoretical and experimental studies demonstrate that parameters such as stacking order, interlayer distance, strain, rotational alignment, and external fields can significantly modulate device performance. Despite these promising developments, challenges remain in large-area synthesis, interface stability, and experimental realization of predicted properties. Addressing these issues through advanced fabrication techniques and systematic experimental validation will be crucial for translating tellurene vdW heterostructures into practical, scalable nanoelectronic technologies.

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