



Research Article

Strain engineering in Ti_2CX_2/WS_2 van der Waals heterostructures: First-principles calculations on mechanical robustness and bandgap tunability



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ABSTRACT

The discovery of tunable electronic and optical properties in two-dimensional (2D) materials has positioned strain engineering as a powerful tool for tailoring material functionalities. While much effort has been made to understand electronic and optical modulation under strain, mechanical reliability and fracture mechanisms remain critical for practical applications. In this study, we investigate the mechanical and electronic responses of Ti_2CX_2/WS_2 ($X = O, F, OH$) van der Waals heterostructures under uniaxial tensile deformation using density functional theory (DFT). The structural stability of the Ti_2CX_2/WS_2 heterostructures ($X = O, F, OH$) was validated by minimal lattice mismatch and confirmed through binding energy and phonon dispersion calculations. Stress-strain analyses revealed distinct mechanical responses compared to individual monolayers, with all heterostructures exhibiting enhanced ultimate tensile strength. Radial distribution function analysis confirmed that the fracture initiates from monolayer bond breaking. Hybrid functional calculations showed that only Ti_2CO_2/WS_2 maintained a strain-tunable bandgap, unlike the metallic behavior in Ti_2CF_2/WS_2 and $Ti_2C(OH)_2/WS_2$. Moreover, strain-induced transitions from type-II to type-I band alignment were observed, highlighting tunable interfacial electronic properties. These findings provide insight into designing robust and tunable 2D heterostructures for flexible and strain-engineered device applications.

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1. Introduction

2D materials have a layered structure with an atomistic thickness, characterized by strong covalent bonds in the in-plane direction and weak van der Waals (vdw) interactions between interlayers. 2D materials have attracted a lot of attention as key materials for the design of next-generation electronic and optical devices because of their unique physical and chemical properties that are derived from these structural features [1–7]. Among various types of 2D materials, transition metal dichalcogenides (TMDs) are undergoing active research due to their promising performance as semiconductors (bandgap value of 1–2 eV) with a high electron mobility [8,9], mechanical flexibility [10], high thermal conductivity [11–14], and tunable bandgaps [15,16]. Among these, materials that use tungsten as the transition metal commonly benefit from cost re-

ductions due to the abundant reserves of tungsten; thus utilized in several applications with promising properties. For example, WS_2 and WSe_2 reveal high carrier mobility and electrical conductivity [17]. In particular, the electronic properties of monolayer WSe_2 exhibit a transition from an indirect to a direct bandgap, along with strong light absorption and high optical nonlinearity. Additionally, they are also appropriate for electronic devices that require nanocomposite materials using TMDs as a filler and versatility because of their high tensile strength and flexibility [18–20].

Meanwhile, MXenes are also one of the representative 2D materials, created by etching the A layer from the MAX phase, which has $M_{n+1}AX_n$ chemical composition [21]. Here, M represents a transition metal, A represents elements of group III or IV, and X is either N or C. Due to the various functional groups and chemical stability, MXenes have the potential to exhibit high mechanical properties [20] and form stable interfaces with other materials [22]. The surface functional groups of MXenes are formed during synthesis or through additional post-synthesis chemical treatments. These surface terminations not only depend on the synthe-

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