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Strain tuning of charge density wave and Mott-insulating states in monolayer VTe₂

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Monolayer vanadium ditelluride (VTe₂) exhibits a $2\sqrt{3} \times 2\sqrt{3}$ charge-density-wave (CDW) order intertwined with a Mott-insulating state. However, the physical mechanisms driving the emergence of the CDW order and the Mott-insulating state are still not well understood. In this study, we systematically investigate the electronic band structure, phonon dispersion, and electron-phonon coupling (EPC) of monolayer VTe₂ under applied biaxial strain. Our results reveal that the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase is metastable in free-standing monolayer VTe₂ but becomes stabilized under compressive strain below $\varepsilon = -2\%$. The formation of the CDW order originates predominantly from strong EPC, rather than from Fermi-surface nesting. The narrowing of the bandwidth due to the CDW order, combined with correlation effects associated with the V 3d orbitals, collectively drive the system into a Mott-insulating state. Furthermore, we find that tensile strain suppresses the CDW order and induces a superconducting state above a critical strain threshold ($\varepsilon = 2\%$). These findings enhance our understanding of correlation physics in monolayer VTe₂ and provide a pathway for strain-engineered manipulation of quantum phases in two-dimensional transition-metal dichalcogenides.

Keywords: charge density wave, Mott-insulating state, superconductivity

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1. Introduction

Layered transition-metal dichalcogenides (TMDs) have attracted significant attention due to their rich physical properties, including charge-density-wave (CDW) order, Mott physics, and superconductivity (SC).^[1–3] The question of whether CDW and SC are competing or compatible remains a long-standing enigma. For instance, in 1T-TaS₂, SC emerges within a textured CDW order, suggesting their coexistence.^[4,5] Conversely, in both 1T-TiSe₂ and 2H-TaS₂, SC is enhanced when the CDW is suppressed.^[6–8] Among TMDs, only a select few exhibit Mott-insulating properties. A prominent example is 1T-TaS₂, where the Mott-insulating state coexists with the so-called “star-of-David” CDW order. Various methods to manipulate the CDW order and induce the collapse of the Mott-insulating state in 1T-TaS₂ have been extensively explored, including high pressure,^[4,9] doping,^[10–13] and interlayer stacking.^[14,15] The realization of two-dimensional (2D) forms of TMDs has prompted a renewed investigation of CDW order and the Mott-insulating state. For instance, monolayer (ML) 1T-TaSe₂ has been identified as a strongly correlated 2D Mott insulator,^[16,17] in contrast to its bulk counterpart, which exhibits metallic properties due to weakened Coulomb interactions from increased elec-

tronic delocalization and screening.

Recently, ML VTe₂ stabilized in the 1T phase has been found to exhibit a coexistence of metallic 4×4 CDW and insulating $2\sqrt{3} \times 2\sqrt{3}$ CDW orders in different regions at low temperatures.^[18–20] In contrast, bulk VTe₂ crystallizes in a monoclinic 1T'' phase with $3 \times 1 \times 3$ periodic lattice distortions.^[21] The emergence of the insulating state accompanied by the $2\sqrt{3} \times 2\sqrt{3}$ CDW order in ML VTe₂ has been attributed to strong V-3d electron correlations, which induce a Mott-insulating state.^[20] Furthermore, previous experiments have also identified 4×1 and 5×1 CDW orders in ML VTe₂.^[19,22–24] The experimentally observed different CDW orders may be ascribed to their sensitivity to external sample conditions. Since ML materials are typically prepared on substrates, substrate-induced strain is an inevitable factor, providing opportunities for tuning the CDW state. To date, the physical mechanisms underlying CDW formation in ML VTe₂ remain poorly understood, and a comprehensive understanding of the interplay between CDW and the Mott state is still elusive. Investigating how strain can modulate the CDW orders and the Mott-insulating state in ML VTe₂ could offer critical insights into controlling correlated quantum states in ML VTe₂.

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In the present work, we employ first-principles calculations to systematically investigate the electronic band structure, phonon dispersion, and electron–phonon coupling (EPC) in ML VTe₂ under biaxial strain. Our comprehensive study reveals that the emergence of diverse CDW orders in ML VTe₂ can be primarily attributed to strong EPC. Furthermore, we demonstrate that strain can significantly modulate the competition between different CDW orders, resulting in distinct electronic ground states. The 4×4 CDW phase is the ground state in free-standing samples, whereas the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase becomes more energetically favorable under compressive strain. Our calculations show that CDW-induced band narrowing, combined with strong correlation effects of the V 3d orbitals, leads to the Mott-insulating state. With increasing tensile strain, the CDW order is gradually suppressed, consequently reducing the Mott gap. Interestingly, once the Mott-insulating state fully collapses, a superconducting state can be induced, with the superconducting transition temperature T_c reaching 8.5 K at 6% tensile strain. These findings not only deepen our understanding of correlation physics in ML VTe₂ but also open new avenues for strain engineering of quantum phenomena in 2D TMDs.

2. Methods

The first-principles calculations based on density functional theory (DFT) were performed using the Vienna *ab initio* simulation package (VASP).^[25,26] The exchange–correlation functional was approximated using the generalized gradient approximation (GGA) formulated by Perdew, Burke, and Ernzerhof (PBE).^[27] To simulate the ML, a 16 Å vacuum layer was introduced to avoid interactions between neighboring slabs. The Coulomb repulsion of V-3d electrons was accounted for using the DFT + *U* method with a Hubbard *U* parameter of 2 eV, consistent with previous studies.^[20] The kinetic-energy cutoff was set to 500 eV, and the Brillouin zone (BZ) was sampled using a Γ -centered grid with a resolution of $0.02 \text{ \AA}^{-1}$ for self-consistent calculations. Transition-state energy differences were calculated using the nudged elastic band (NEB) method,^[28,29] as implemented in the VTST code.^[30] The phonon dispersion spectrum for the 1T structure was calculated using the Quantum ESPRESSO package^[31] within density functional perturbation theory (DFPT).^[32] A $10 \times 10 \times 1$ *q*-point grid and a $20 \times 20 \times 1$ *k*-point grid were employed to sample the BZ. The wave-function and charge-density energy cutoffs were set to 100 Ry and 700 Ry, respectively. The biaxial strain was simulated by adjusting the lattice parameters along the *ab* axes. The strain magnitude ε is defined as $(a - a_0)/a_0 \times 100\%$, where positive (negative) values of ε denote biaxial tensile (compressive) strain applied to the system.

3. Results and discussion

At room temperature, ML VTe₂ crystallizes in a high-symmetry octahedral 1T structure (Fig. 1(a)), where hexagonally arranged V atoms are sandwiched between two layers of Te atoms in an octahedral coordination. Upon cooling to lower temperatures, ML VTe₂ exhibits two distinct CDW states: a metallic 4×4 CDW order and an insulating $2\sqrt{3} \times 2\sqrt{3}$ CDW order.^[18,20] The low-symmetry CDW superstructure typically evolves from the high-symmetry phase, with distortions introduced by underlying instability. When the temperature drops below the CDW transition temperature, the material undergoes lattice distortion, leading to atomic rearrangement and cluster formation. To investigate the characteristics of ML VTe₂, we simulated the superstructures of the 4×4 and $2\sqrt{3} \times 2\sqrt{3}$ CDW orders. In the 4×4 superstructure, 13 V atoms are arranged in a “star of David” cluster (Fig. 1(c)). Conversely, in the $2\sqrt{3} \times 2\sqrt{3}$ superstructure, 12 V atoms are arranged into a truncated triangle-shaped cluster (Fig. 1(d)). The lattice distortion is attributed to the dimerization of V atoms accompanied by the vertical bulge of the Te atoms.

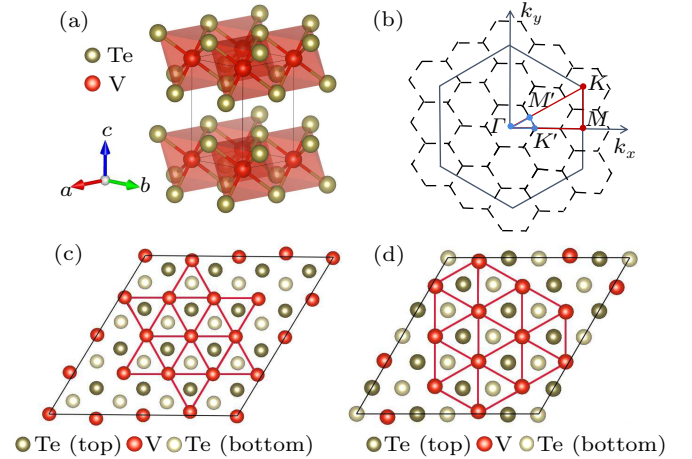


Fig. 1. (a) Crystal structure of bulk 1T-VTe₂. Red and brown spheres represent V and Te atoms, respectively. (b) BZs of monolayer 1T-VTe₂ unit cell (solid line) and $2\sqrt{3} \times 2\sqrt{3}$ superstructure (dashed line), in which the high-symmetry *k*-points are labeled by red and blue points, respectively. Superstructures of the (c) 4×4 and (d) $2\sqrt{3} \times 2\sqrt{3}$ CDW orders. Red lines indicate atomic bonds whose lengths change due to the CDW distortions. Here, the V–V bond lengths decrease by $\sim 6\%$ compared with those in the high-symmetry 1T phase.

Our calculations show that the structural optimization of the $2\sqrt{3} \times 2\sqrt{3}$ superstructure, incorporating a Hubbard *U* value of 2 eV, revealed a $\sim 6\%$ reduction in the bond length between neighboring V atoms compared to the ideal 1T structure. The result is consistent with previous scanning tunneling spectroscopy experimental observations.^[20] We calculated the electronic band structures of prototype 1T, 4×4 CDW, and $2\sqrt{3} \times 2\sqrt{3}$ CDW phases of ML VTe₂. As shown in Figs. 2(a)–2(c), both the prototype 1T and the 4×4 CDW phases exhibit metallic behavior, while a full gap opens for the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase. The electron bands near the

Fermi level are contributed mainly by the V-3d orbitals. For the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase, the CDW order narrows the bandwidth, allowing the strong correlation effects of the V-3d orbitals to open a Mott gap and induce an insulating state, in agreement with previous experimental results.^[18,20] This physical mechanism can be captured in supplemental Fig. S2(f). For the CDW state, the Mott gap opens between the upper and lower Hubbard bands (UHB and LHB), due to the electron–electron interaction. Therefore, this indicates that the CDW distortion and the strong electron–electron interaction

play an essential role in initiating the Mott gap opening. The Mott physics in the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase of ML VTe₂ is different from other widely explored TMDs, such as ML 1T-TaS₂, 1T-TaSe₂, and 1T-NbSe₂.^[16,33–36] In those materials, the “star of David” cluster hosts an odd number (13) of d-electrons per CDW superstructure and an isolated half-filled narrow band. In contrast, ML VTe₂ nominally hosts an even number (12) of d-electrons. The distinction suggests that the above-mentioned Mott-insulating model may not directly apply to VTe₂.

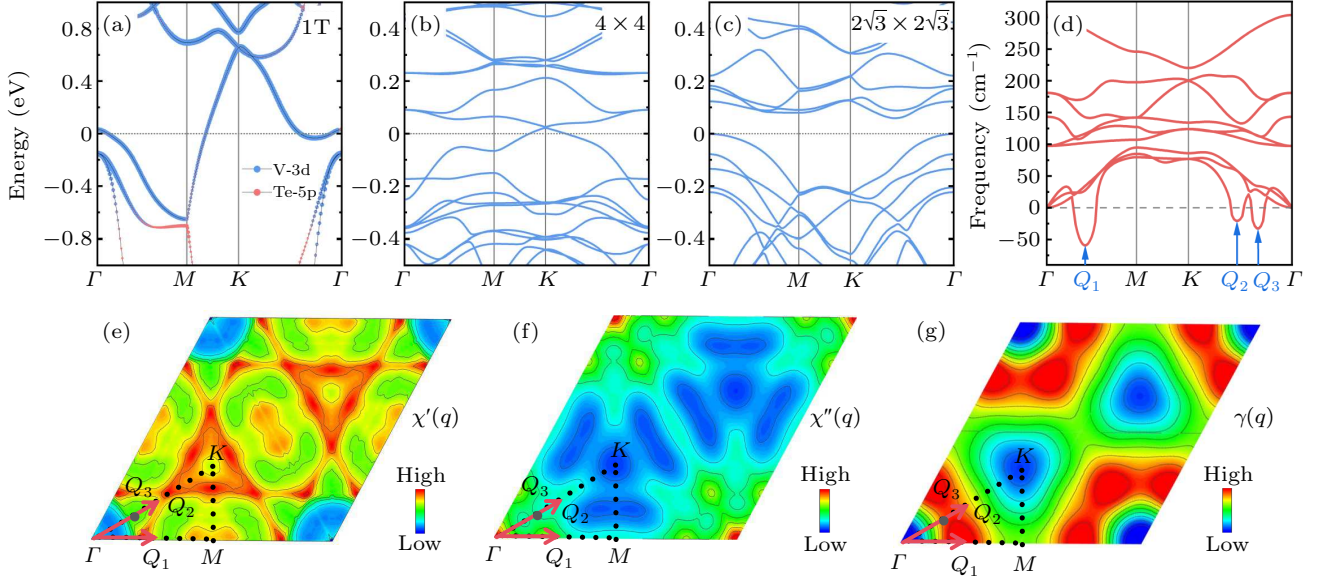


Fig. 2. Calculated band structures of ML VTe₂ in the (a) prototype 1T, (b) 4×4 CDW, and (c) $2\sqrt{3} \times 2\sqrt{3}$ CDW phases using the DFT + U method with $U = 2$ eV. (d) Phonon dispersion spectrum of ML VTe₂ with the high-symmetry 1T structure, where Q_1 , Q_2 , and Q_3 denote three distinct soft phonon modes, indicated by blue arrows. (e) The real and (f) imaginary parts of the electron susceptibility cross-section of ML VTe₂ in the $q_z = 0$ plane, where Q_1 and Q_2 are indicated by pink arrows, while Q_3 is marked by a gray point. (g) shows the phonon linewidth of the lowest phonon mode of ML VTe₂ in the $q_z = 0$ plane.

To investigate the physical origin of the CDW in ML VTe₂, we first calculated the phonon spectrum of its high-temperature 1T structure. For materials exhibiting CDW orders at low temperatures, the phonon spectrum of the high-temperature phase typically displays an instability near the CDW wave vector Q_{CDW} .^[37] In real space, the corresponding atomic displacements give rise to the low-temperature CDW superstructure. In Table S1 of the supplemental material, we list the Q_{CDW} values of various CDW superstructures. The calculated phonon spectrum in Fig. 2(d) shows three distinct soft phonon modes, labeled Q_1 , Q_2 , and Q_3 . The phonon instability at the wave vector $Q_1 \sim \frac{1}{2}\Gamma M$ is related to the 4×4 CDW order, while the instability at $Q_2 \sim \frac{1}{2}\Gamma K$ is associated with the $2\sqrt{3} \times 2\sqrt{3}$ CDW order. In contrast, the instability at $Q_3 \sim \frac{1}{3}\Gamma K$ can be attributed to the $\sqrt{19} \times \sqrt{19}$ CDW order (see supplemental Fig. S2), which has previously been observed experimentally in 1T-NbTe₂ and 1T-TaTe₂,^[38–40] both of which are structurally analogous to 1T-VTe₂.

Since the EPC plays an important role in the formation of CDW,^[41,42] we calculate the phonon linewidth γ , which is

directly related to the strength of the EPC. The q - and phonon mode ν -resolved linewidth $\gamma_{q\nu}$ is defined as

$$\gamma_{q\nu} = 2\pi\omega_{q\nu} \sum_{ij} \int \frac{d^3k}{\Omega_{\text{BZ}}} |g_{q\nu}(k, i, j)|^2 \times \delta(\epsilon_{q,i} - \epsilon_F) \delta(\epsilon_{k+q,i} - \epsilon_F). \quad (1)$$

Here $g_{q\nu}(k, i, j)$ is the EPC matrix element, given by

$$g_{q\nu}(k, i, j) = \left(\frac{\hbar}{2M\omega_{q\nu}} \right)^{1/2} \langle \psi_{i,k} | \frac{dV_{\text{SCF}}}{d\hat{u}_{q\nu}} \hat{\xi}_{q\nu} | \psi_{j,k+q} \rangle, \quad (2)$$

where ψ is the electronic wave function, V_{SCF} is the Kohn–Sham potential, $\hat{u}$ is the atomic displacement, and $\hat{\xi}$ is the phonon eigenvector. The results shown in Fig. 2(g) indicate that the maxima of γ occur at Q_1 and Q_2 , but not at Q_3 . This suggests that EPC interactions play a dominant role in the formation of the 4×4 and $2\sqrt{3} \times 2\sqrt{3}$ CDW orders in ML VTe₂.

Another perspective on the driving force of CDW formation is Fermi surface (FS) nesting, which can be evaluated quantitatively by calculating the electron

susceptibility.^[40,43,44] The real part of the electron susceptibility, χ' , is defined as

$$\chi'(q) = \sum_k \frac{f(\epsilon_k) - f(\epsilon_{k+q})}{\epsilon_k - \epsilon_{k+q}}, \quad (3)$$

where $f(\epsilon_k)$ is the Fermi–Dirac distribution function. The imaginary part of the electron susceptibility, χ'' , is given by

$$\chi''(q) = \sum_k \delta(\epsilon_k - \epsilon_F) \delta(\epsilon_{k+q} - \epsilon_F). \quad (4)$$

Here, χ' reflects the stability of the electronic subsystem, while χ'' is referred to as the “nesting function.” If the CDW order arises from FS nesting, both χ' and χ'' should exhibit maxima at Q_{CDW} . However, our calculations for ML VTe₂, shown in Figs. 2(e) and 2(f), reveal that neither χ' nor χ'' displays maxima at the wave vectors Q_1 , Q_2 , or Q_3 . This observation suggests that FS nesting does not play a significant role in the formation of the CDW orders in ML VTe₂. Our calculations of the phonon linewidth γ obtained from DFPT, combined with the electron susceptibility, indicate that EPC rather than FS nesting governs CDW formation in ML VTe₂.

To further evaluate the stability of potential CDW phases from an energetic perspective, we investigate how biaxial strain affects the formation energy of the 4×4 , $2\sqrt{3} \times 2\sqrt{3}$, and $\sqrt{19} \times \sqrt{19}$ superstructures. The CDW formation energy is defined as the total energy of a CDW phase relative to that of the high-symmetry 1T phase, i.e., $E_{\text{CDW}} - E_{1T}$. A negative CDW formation energy indicates that the CDW structure is energetically favorable, with more negative values corresponding to greater stability. As shown in Fig. 3(a), under compressive strain, the CDW formation energy becomes negative, and its absolute value progressively increases, indicating enhanced stability of the CDW phases. In contrast, under tensile strain, the formation energy approaches zero or even becomes positive, suggesting that the CDW order is suppressed. This conclusion is further supported by analyzing the displacements of V atoms in potential CDW phases under different biaxial strains, as shown in supplemental Fig. S2. The distortion of V atoms decreases under tensile strain, correlating with an inhibitory effect on CDW formation. Collectively, these findings demonstrate that compressive strain promotes CDW formation in ML VTe₂, while tensile strain suppresses it.

In free-standing ML VTe₂ without strain, the 4×4 CDW phase exhibits the largest absolute formation energy, while that of the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase shows the smallest. This implies that the 4×4 CDW phase is the most stable in free-standing ML VTe₂ and that the $\sqrt{19} \times \sqrt{19}$ CDW phase may be unstable. The absence of experimental observations of the $\sqrt{19} \times \sqrt{19}$ CDW phase until now could be attributed to this instability. Furthermore, the $2\sqrt{3} \times 2\sqrt{3}$ superstructure likely represents a metastable phase. However, under compressive

strain exceeding 2%, a notable transition occurs: The absolute formation energy of the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase surpasses that of the 4×4 CDW phase, indicating a shift in ground state stability. This suggests that the experimentally observed $2\sqrt{3} \times 2\sqrt{3}$ CDW phase in strained ML VTe₂ samples could be attributed to such compressive strain effects. To further explore the transition dynamics between the CDW phases, we employed the NEB method to evaluate the energy barrier from the initial $2\sqrt{3} \times 2\sqrt{3}$ CDW phase to the final 4×4 CDW phase. The energy difference is defined as $\Delta E = E_{2\sqrt{3} \times 2\sqrt{3}} - E_{\text{transition}}$. As shown in Fig. 3(b), though the 4×4 CDW phase is energetically favorable, the system may remain locked in the metastable $2\sqrt{3} \times 2\sqrt{3}$ CDW phase in free-standing ML VTe₂ without strain due to the high activation barrier (~ 8 meV). Transition to the more stable 4×4 CDW phase requires sufficient energy to overcome the hill in the free energy space and stabilize the system in a new local valley.

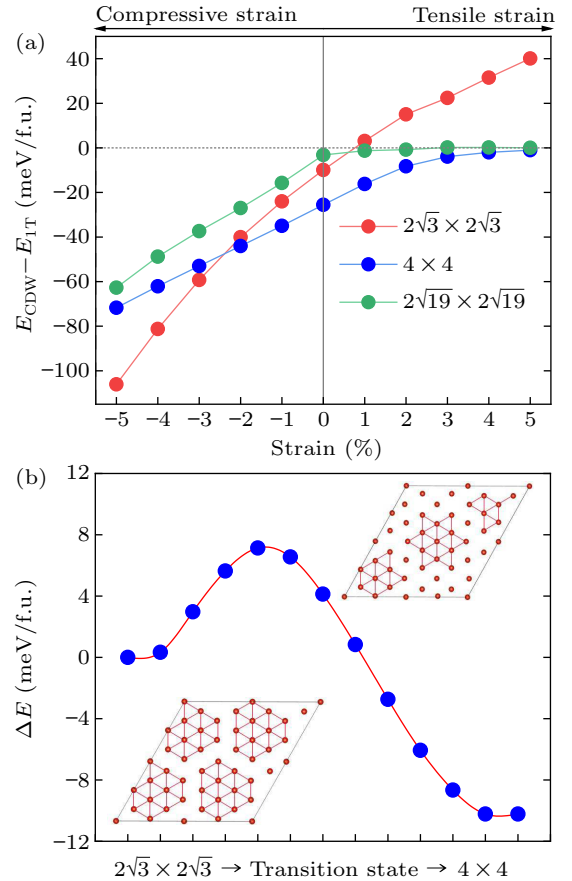


Fig. 3. (a) CDW formation energies of potential CDW superstructures in ML VTe₂ as a function of biaxial strain. (b) Energy difference for the transition from the initial $2\sqrt{3} \times 2\sqrt{3}$ CDW phase to the final 4×4 CDW phase. Insets show schematic illustrations of the $2\sqrt{3} \times 2\sqrt{3}$ and 4×4 superstructures.

Further analysis of the electronic states under strain reveals significant differences. For the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase, the Mott gap increases upon compressive strain (Figs. 4(a)–4(c)). We find that applying compressive strain reduces the lattice parameters and enhances the atomic displacement, thereby

enhancing the CDW distortion. Consequently, the bandwidth narrows and the Mott gap gradually widens. Conversely, tensile strain suppresses the CDW distortion, leading to a reduction in the Mott gap. Notably, when tensile strain exceeds 3%, the energy gap disappears completely (Fig. 4(e)), indicating

the collapse of the Mott-insulating state. In contrast to the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase, the metal-characteristic energy band of the 4×4 CDW phase remains relatively insensitive to strain variation (supplemental Fig. S3), demonstrating its robustness against external mechanical perturbations.

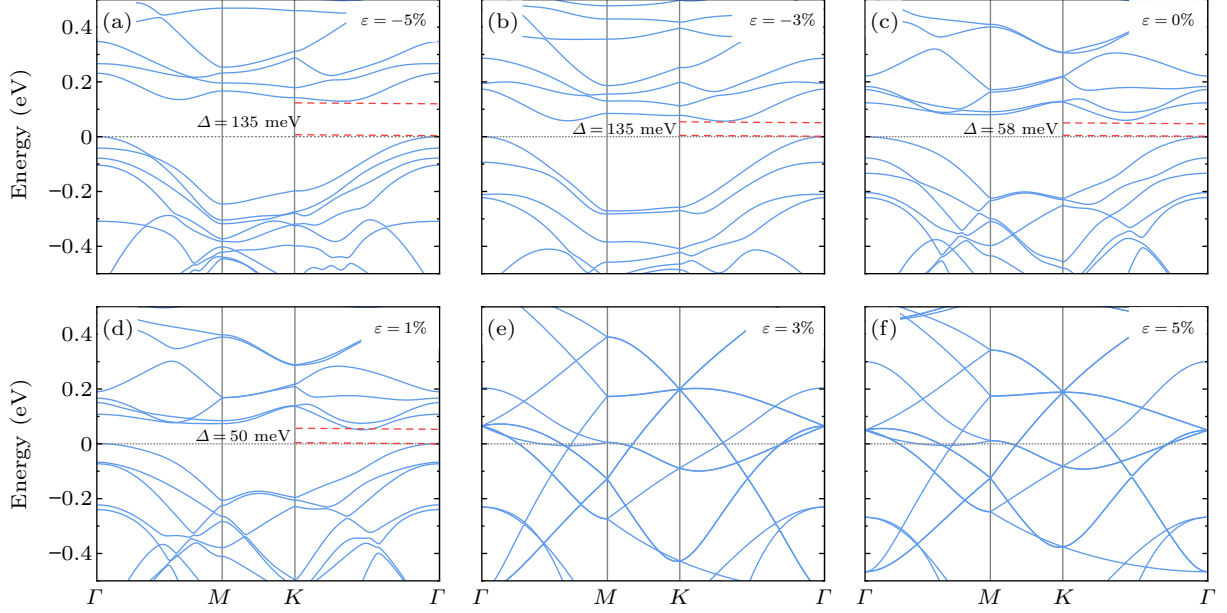


Fig. 4. Electronic band structures of the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase under biaxial strain: (a) and (b) for compressive strain, (c) at zero strain, and (d)–(f) for tensile strain. The top of the valence band is set to zero. Red dashed lines in (a)–(d) indicate the energy gap Δ , which systematically decreases as the magnitude of biaxial tensile strain increases.

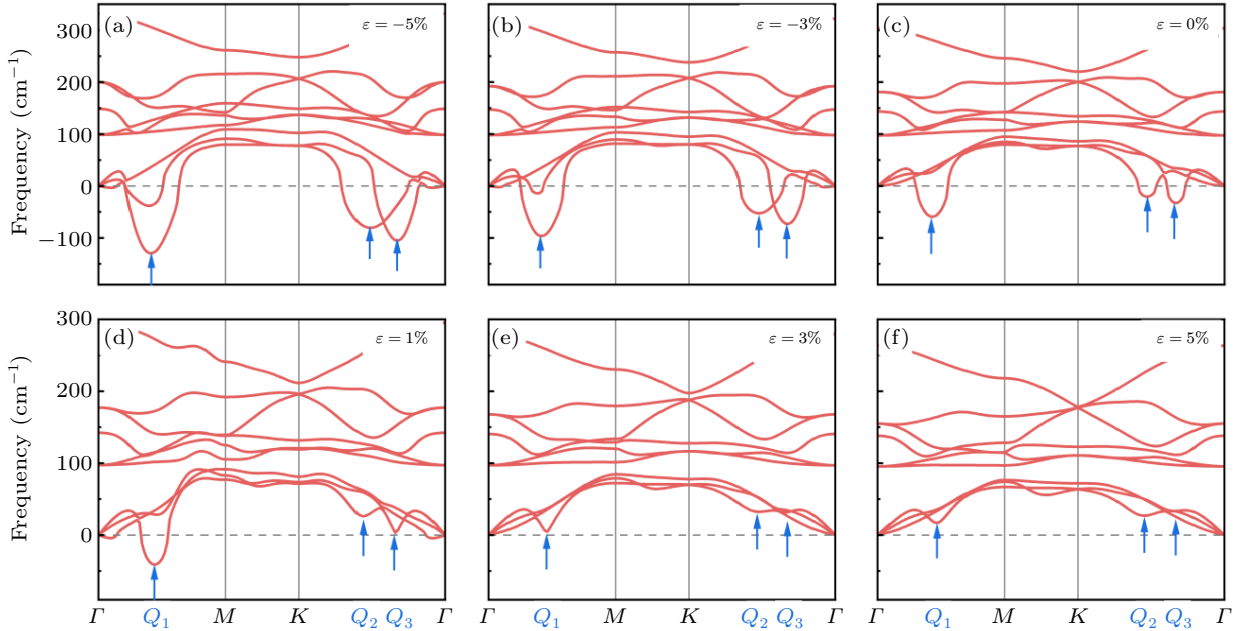


Fig. 5. Phonon dispersion spectra of ML VTe₂ in the high-symmetry 1T phase under biaxial strain: (a) and (b) for compressive strain, (c) at zero strain, and (d)–(f) for tensile strain, where Q_1 , Q_2 , and Q_3 denote three distinct soft phonon modes, indicated by blue arrows.

Next, we calculate the phonon spectrum to evaluate the stability of the high-symmetry 1T structure under various biaxial strains. It is well-established that imaginary phonon frequencies at a specific wave vector Q_{CDW} indicate lattice restructuring associated with a CDW superstructure characterized by Q_{CDW} . Conversely, the absence of imaginary frequen-

cies in the phonon spectrum implies structural stability relative to the CDW superstructure. Figure 5 shows the phonon dispersion spectra of ML VTe₂ with undistorted 1T structure under different strains. Compared to the strain-free case (Fig. 5(c)), the acoustic branches at wave vectors Q_1 , Q_2 , and Q_3 exhibit increased softening and become less stable as compressive

strain increases. Under tensile strain, however, these softened acoustic branches become more stable, suggesting that CDW distortions are suppressed as tensile strain increases. The phonon spectrum of the $2\sqrt{3} \times 2\sqrt{3}$ CDW supercell exhibits no imaginary frequencies under compression ($\varepsilon = -3\%$), further reinforcing the above conclusion (supplemental Fig. S5). Interestingly, our findings align with those observations in $1H$ -TaSe₂,^[45] yet they present a contrasting scenario to previous studies on $1T$ -TaS₂^[9] and $1T$ -TiSe₂.^[46] This divergence underscores the unique mechanical and electronic properties of ML VTe₂ under strain. Additionally, we also find that phonon spectra exhibit small imaginary frequencies near the Γ point

under compressive and moderate tensile strains. Such a phenomenon is similar to the case of the long-wavelength rippling triggered by light-induced electron–hole excitation in 2D boron nitride (BN) as previously reported by Liu *et al.*^[47] As can be seen in Fig. S6 of supplemental material, our calculations of the hole-doped phonon spectra under different external strains exhibit inconsistent trends, which complicates the determination of an analogous mechanism in ML VTe₂. Further theoretical and experimental investigations are needed to clarify the physical mechanism of the small imaginary frequencies near the Γ point in ML VTe₂.

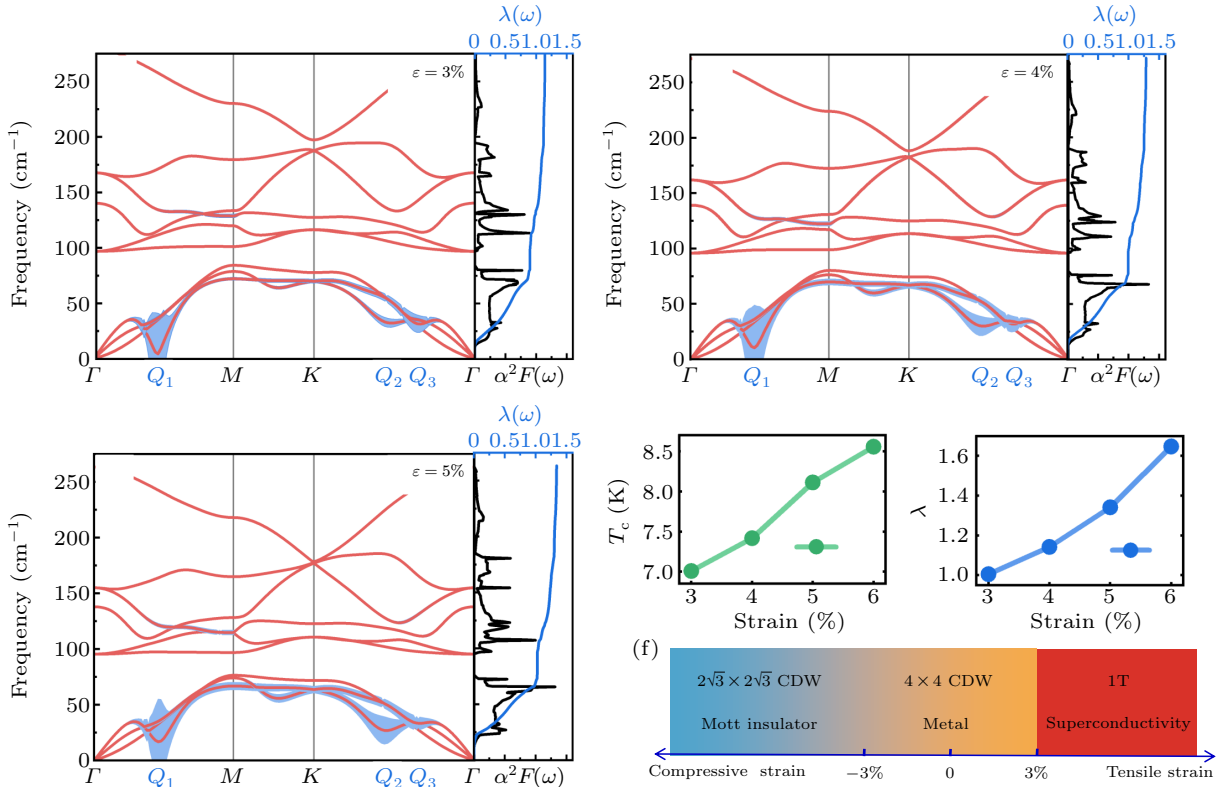


Fig. 6. Phonon dispersion spectra weighted by the magnitude of EPC strength λ_{qv} under biaxial tensile strains of (a) 3%, (b) 4%, and (c) 5%. The Eliashberg spectral function $\alpha^2 F(\omega)$ (black) and the integrated EPC strength $\lambda(\omega)$ (blue) are plotted on the right. (d) and (e) Calculated superconducting transition temperature T_c and EPC constant λ as a function of biaxial tensile strain (3%–6%). (f) Schematic diagram illustrating the structural and electronic state changes in ML VTe₂ under varying biaxial strain.

SC typically emerges after the suppression of CDW or Mott-insulating states, as observed in most TMDs.^[4,48,49] Here, we investigate the possibility of a superconducting state in ML VTe₂ under large tensile strain, where both CDW and Mott-insulating states are completely suppressed. To evaluate SC, we calculated the Eliashberg spectral function $\alpha^2 F(\omega)$ and EPC strength $\lambda(\omega)$ using the following expressions:

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(E_F)} \sum_{qv} \delta(\omega - \omega_{qv}) \frac{\gamma_{qv}}{\hbar \omega_{qv}}, \quad (5)$$

$$\lambda(\omega) = \sum_{qv} \lambda_{qv} = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega. \quad (6)$$

The calculated $\alpha^2 F(\omega)$ and integrated $\lambda(\omega)$ are plotted on

the right side of phonon spectra in Figs. 6(a)–6(c). Additionally, we present the calculated EPC strength at each wave vector and phonon mode, λ_{qv} . Notably, the phonon branch with the CDW-type softening mode exhibits the largest electron–phonon coupling. Next, we calculate the superconducting transition temperature T_c using the Allen–Dynes–modified McMillan formula^[50]

$$T_c = \frac{\omega_{\log}}{1.2} \exp \left(-\frac{1.04(1 + \lambda)}{\lambda - \mu^* - 0.62\lambda\mu^*} \right), \quad (7)$$

where the Coulomb pseudopotential μ^* is set to a typical value of 0.1.^[42,51] We estimated the T_c and λ of ML VTe₂ under varying tensile strain and show the results in Figs. 6(d) and

6(e). Both T_c and λ exhibit a monotonic increase with increasing tensile strain. Specifically, at $\varepsilon = 3\%$, we determine $T_c = 7$ K and $\lambda = 1.1$. These values reach their maximum at $\varepsilon = 6\%$ with $T_c = 8.5$ K and $\lambda = 1.6$. However, we should note that further strain ($\varepsilon \geq 7\%$) triggers pronounced imaginary phonon branches along high-symmetry paths ($\Gamma \rightarrow K$) (see Fig. S7 of supplemental material), indicating a structural phase transition or lattice collapse. Our results indicate that tensile stress suppresses the CDW order and Mott gap in the $2\sqrt{3} \times 2\sqrt{3}$ CDW state, while simultaneously enhancing superconducting properties. In contrast, compressive strain notably strengthens the CDW state. These results demonstrate that biaxial strain provides an effective method of manipulating the CDW, Mott-insulating, and superconducting states in ML VTe₂, as summarized schematically in Fig. 6(f). This strain-dependent behavior underscores the potential of mechanical deformation as a flexible tool for controlling the electronic properties of ML VTe₂ with correlated electron states.

4. Conclusion

In conclusion, we have systematically investigated the physical origins of CDW orders and the effects of biaxial strain on CDW phases and electronic states in ML VTe₂. Our results reveal the critical role of EPC in driving the formation of CDW in ML VTe₂. The 4×4 CDW phase represents the ground state in free-standing ML VTe₂, while the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase becomes more energetically favorable under compressive strain. The narrowing of the bandwidth due to the CDW order, together with the strong correlation effect of the V-3d orbital, results in the opening of a Mott gap in the $2\sqrt{3} \times 2\sqrt{3}$ CDW phase. Our calculations of the band structure and phonon spectra under various biaxial strains indicate the profound effects of strain on the electronic properties. Compressive strain significantly enhances the CDW order and the associated Mott-insulating state, while tensile strain suppresses the CDW order, thereby facilitating the emergence of a potential SC state. Our work highlights the potential of strain engineering as a powerful tool for manipulating phase transitions in ML VTe₂. The coexistence of the CDW, Mott-insulating states, and strain-induced superconducting state in ML VTe₂ presents promising opportunities for exploring the intricate interplay between distinct quantum states.

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