

Strain-induced charge-density-wave phase transitions in magnetic kagome FeGe

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FeGe is the only known kagome metal hosting the coexistence of long-range magnetic order and charge-density-wave (CDW) order, making it an exceptional platform for studying spin-charge-lattice entanglement. Despite extensive experimental and theoretical efforts, the microscopic origin of the CDW in FeGe remains under active debate. In this work, we reveal how in-plane tensile strain reshapes the hierarchy of competing CDW orders in the antiferromagnetic kagome metal FeGe. First-principles phonon calculations uncover two Kohn-anomaly-induced incommensurate CDWs under strain, while slight electron correlations suppress these modes and instead lead to unconventional correlation-driven CDW phases. Notably, a previously unreported fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW emerges from the softened H -point phonon mode. Total-energy analyses establish a strain-induced phase transition sequence: $2 \times 2 \times 2 \rightarrow \sqrt{3} \times \sqrt{3} \times 2 \rightarrow$ fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ at strains of $\sim 0.6\%$ and $\sim 2.4\%$, respectively, while a small $U = 0.2$ eV will reduce the required strain to $\sim 0.2\%$ and $\sim 1.8\%$, respectively. These results demonstrate the coexistence of electron-phonon-driven and correlation-driven CDW mechanisms, positioning strained FeGe as a powerful platform for probing strongly coupled spin-charge-lattice entanglement in correlated magnetic kagome systems.

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I. INTRODUCTION

The kagome lattice has emerged as a fertile platform for exploring the interplay among geometry, strong correlations, and topology. Its characteristic electronic structure features, such as Dirac crossings, flat bands, and Van Hove singularities (VHSs) [1–4], give rise to a wide variety of emergent quantum phenomena, including quantum spin liquid [5], nematicity [6], anomalous Hall effect [7–9], superconductivity [10–13], and charge-density-wave (CDW) order [14–18]. Among these phenomena, CDW order refers to a spontaneous modulation of the electronic charge density accompanied by a periodic lattice distortion, reflecting a strong coupling between electronic and lattice degrees of freedom [19,20].

Recently, the kagome metals AV_3Sb_5 ($A = Cs, K, Rb$) have attracted considerable attention due to the interplay between nontrivial band topology, unconventional CDW order, and superconductivity [10–16,21–26]. Despite intensive investigations, AV_3Sb_5 family lacks intrinsic magnetism, thereby limiting a direct understanding of how spin degrees of freedom participate in the CDW formation. This limitation motivates the exploration of kagome system in which magnetism,

electronic correlations, and lattice degrees of freedom are inherently intertwined.

In this context, the magnetic kagome metal FeGe provides a unique and compelling platform. FeGe exhibits an A-type antiferromagnetic (AFM) order below the Néel temperature $T_N \approx 410$ K, characterized by ferromagnetic kagome layers stacked antiferromagnetically along the c axis [27]. Upon further cooling below $T_{CDW} \approx 110$ K, neutron scattering experiments revealed the emergence of a triple- Q CDW at the $M(0.5, 0, 0)$, $A(0, 0, 0.5)$, and $L(0.5, 0, 0.5)$ points, accompanied by an enhancement of the ordered magnetic moments [17,18,28]. Complementary real-space evidence from scanning tunneling microscopy further reveals a 2×2 CDW below T_{CDW} . Detailed comparisons with first-principles simulations suggest that the observed CDW is predominantly associated with distortions of the Ge sublattice rather than the Fe kagome network [29,30]. To date, FeGe remains the only known kagome material in which long-range magnetic order and CDW modulation coexist, rendering it an exceptional system for investigating spin-charge-lattice intertwined physics.

First-principles calculations suggest that the experimentally observed CDW in FeGe corresponds to a $2 \times 2 \times 2$ superstructure associated with a pronounced Ge-1 dimerization [28,31]. However, the microscopic mechanism responsible for stabilizing this CDW remains unresolved, indicating that FeGe may host an unconventional ordering phenomenon beyond standard weak-coupling descriptions in terms of Fermi-surface nesting [19,20,32–34] or electron-phonon-driven Kohn anomalies [32–36]. A typical Kohn anomaly is characterized by a pronounced phonon softening

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at a specific CDW wave vector in the phonon spectrum. In first-principles phonon calculations, as the Fermi smearing temperature (introduced through the Fermi-Dirac broadening factor) is gradually increased from low to high values, the phonon instability can evolve from an unstable region with imaginary frequencies to a stable region without imaginary frequencies. The wave vector at which the imaginary phonon frequency appears corresponds to the CDW wave vector [37,38].

Several competing scenarios have been proposed. Angle-resolved photoemission spectroscopy (ARPES) measurements combined with density functional theory (DFT) calculations reveal that antiferromagnetic band splitting shifts the VHSs at the M point toward the Fermi level, suggesting that VHS-enhanced electronic nesting could promote CDW formation [17,18]. In contrast, DFT plus Hubbard U (DFT + U) phonon calculations indicate that enhanced electronic correlations and magnetic moments can induce phonon softening at the L point, consistent with satellite peaks observed in neutron diffraction experiments, highlighting a possible dominant role of spin-phonon coupling [28,31]. However, the magnetic moments obtained within DFT + U are significantly overestimated compared with experimental values, raising concerns regarding the quantitative validity of this description. Moreover, the nesting function derived from DFT exhibits a peak in the electronic susceptibility at the K point, which is inconsistent with the experimentally observed CDW modulation vectors located near the M , L , and A points [39]. Taken together, these results suggest that the CDW in FeGe is an unconventional, correlation-driven order [28] that cannot be adequately explained by conventional Fermi-surface nesting or Kohn-anomaly mechanisms [19,20,32–36].

Beyond ambient pressure, high-pressure experiments and first-principles calculations on FeGe reveal the emergence of a competing $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase that destabilizes the original $2 \times 2 \times 2$ CDW order [40,41]. Notably, both CDW phases involve a large Ge-1 dimerization along the c axis, suggesting that lattice distortions along this direction play a crucial role in stabilizing the CDW landscape. This observation naturally raises the question of how strain influences the stability and competition of CDW phases in FeGe.

In this study, we systematically investigated how tensile strain along the ab axis influences the evolution and competition of multiple CDW phases in FeGe. We first examine phonon spectra calculated with different Fermi smearing temperatures to probe electronic thermal broadening, and find that under 2.8% tensile strain, two pronounced Kohn-anomaly-related soft modes emerge near the high-symmetry H point. Analysis of their CDW propagation vectors reveals noninteger components, suggesting possible formation of incommensurate CDW states driven by electron-phonon coupling. We then investigate the effect of electronic correlations by varying the Hubbard U and found that two distinct phonon softenings develop at the high-symmetry A and H points, while the Kohn-anomaly-related soft modes are suppressed. This observation suggests a competition between conventional electron-phonon-coupled CDWs and unconventional correlation-driven CDWs. Further analysis of the softened phonon mode at the H point predicts a fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase. Subsequently, total-energy and

magnetic-moment calculations reveal a cascade of strain-induced phase transitions: from the $2 \times 2 \times 2$ CDW phase to the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase, and finally to the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ phase. Our findings demonstrate strain-induced competition among multiple CDW phases in FeGe and establish it as a promising platform for investigating strongly coupled spin-charge-lattice systems.

II. COMPUTATIONAL METHODS

First-principles calculations were performed using the Vienna *ab initio* simulation package [42,43] based on DFT, with the exchange-correlation functional treated within the generalized gradient approximation of the Perdew-Burke-Ernzerhof [44]. The DFT + U calculations were carried out using the simplified rotationally invariant approach [45] as commonly adopted in previous first-principles studies of FeGe [28,40,46]. Regarding the on-site Hubbard U value, we have tested U values ranging from 0 to 3 eV and found that the experimentally observed stable $2 \times 2 \times 2$ CDW phase [17] at ambient pressure is reproduced for $U \leq 0.3$ eV. We therefore take $U = 0.2$ eV as a representative value in this article, which also enables direct comparison with previous high-pressure studies [40]. Further details are provided in Fig. S4 of the Supplemental Material [47]. The plane-wave energy cutoff was set to 500 eV. A Γ -centered k -point grid of $12 \times 12 \times 7$, $6 \times 6 \times 7$, $7 \times 7 \times 7$, and $7 \times 7 \times 7$ was used for the calculations of the pristine phase, the $2 \times 2 \times 2$ CDW phase, the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase, and the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase, respectively. Starting from the experimental lattice parameters $a = b = 4.985$ Å and $c = 4.048$ Å of FeGe [17,48], we simulate the effect of strain on the A-type AFM configuration by elongating or compressing the in-plane lattice constants a and b with the lattice constant c relaxed. The internal atomic positions in all CDW phases were relaxed until the residual forces were below 0.001 eV/Å. Phonon calculations were performed using the finite displacement method within the PHONOPY package [49,50], employing a $2 \times 2 \times 2$ supercell relative to the primitive cell. The crystal structures were visualized using the VESTA software [51,52].

III. RESULTS AND DISCUSSION

Kagome FeGe crystallizes in a hexagonal structure with space group $P6/mmm$ (No. 191) and experimental lattice parameters of $a = b = 4.985$ Å and $c = 4.048$ Å [17,48]. Along the c axis, the structure consists of alternating Fe₃Ge kagome layers and Ge honeycomb layers. Within each Fe₃Ge kagome layer, Ge-1 atoms occupy the centers of kagome stars formed by Fe atoms, as illustrated in Figs. 1(a) and 1(b). Below the Néel temperature $T_N \approx 410$ K [27], FeGe adopts an A-type AFM configuration, in which the magnetic moments of Fe atoms in adjacent kagome layers are aligned antiparallel along the c axis, with a magnetic moment of approximately $1.5\mu_B$ per Fe atom [17]. Upon further cooling below the CDW transition temperature $T_{CDW} \approx 110$ K [17,18], the magnetic moments in FeGe are enhanced, and a $2 \times 2 \times 2$ CDW phase emerges, accompanied by a large dimerization of the Ge-1 atoms, as shown in Fig. 1(c). When FeGe is subjected to

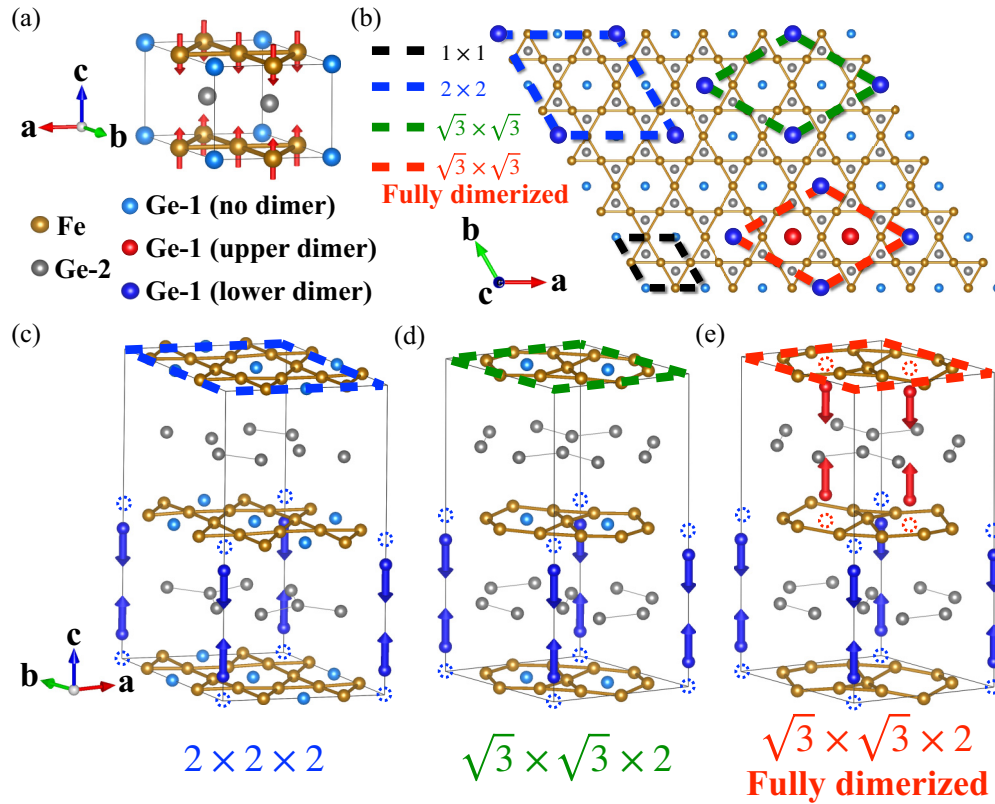


FIG. 1. (a) Pristine FeGe structure exhibiting a hexagonal lattice with space group $P6/mmm$. Gold spheres denote Fe atoms. Ge-1 atoms are color coded as follows: light blue for nondimerized, red for upper large dimers, and dark blue for lower large dimers. Silver spheres represent Ge-2 atoms. Red arrows indicate magnetic moment directions, corresponding to the A-type AFM configuration. (b) Top view of the Fe sublattice, showing the characteristic kagome star pattern. The primitive cell is indicated by the black dashed rhombus. The blue, green, and red dashed rhombuses denote the $2 \times 2 \times 2$, $\sqrt{3} \times \sqrt{3} \times 2$, and fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phases, respectively. Enlarged red and dark blue spheres highlight the upper and lower Ge-1 dimer sites. Panels (c)–(e) show the structures of $2 \times 2 \times 2$, $\sqrt{3} \times \sqrt{3} \times 2$, and fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phases. Red and dark blue arrows indicate the dimerization directions of the upper and lower large Ge-1 dimers, respectively. All CDW structures exhibit large Ge-1 dimerization, accompanied by subtle distortions of other atomic sites.

uniform pressure, a $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase is induced, as illustrated in Fig. 1(d).

To study the strain effect on the CDW formation in FeGe, we optimize the c -axis lattice constant under tensile strain along the ab axis. As shown in Fig. S1 of the Supplemental Material [47], slight elongation along the ab axis leads to the compression of the c -axis lattice constant, effectively preserving the overall volume of the unit cell. To examine the structural stability of FeGe under lateral tensile strain, we calculate the phonon spectra of the pristine FeGe phase at zero, 1.1%, and 2.8% tensile strain along the ab axis, as shown in Fig. 2. At zero strain, variations in Fermi smearing temperature have a negligible effect on phonon spectra in Fig. 2(a), and no characteristic Kohn anomalies associated with CDW formation are observed, consistent with previous reports [28]. Here, a characteristic Kohn anomaly refers to the softening in the DFT phonon spectrum at the CDW wave vector. Moreover, the DFT phonon softening is suppressed as the Fermi smearing temperature increases, reflecting the evolution of the CDW phase transition [37,38].

As strain increases to 1.1% and 2.8%, the FeGe lattice remains dynamically stable, as shown in Figs. 2(b) and 2(c), respectively. With increasing strain, two distinct Kohn

anomalies gradually develop near the H point, corresponding to two incommensurate charge-density-wave (ICDW) modes, labeled as $\mathbf{Q}_{\text{ICDW1}} = (0.24, 0.38, 0.5)$ and $\mathbf{Q}_{\text{ICDW2}} = (0.28, 0.28, 0.5)$. These results indicate that strain enhances the electron-phonon interaction and leads to the emergence of Kohn anomalies, which fundamentally differs from the previously reported spin-phonon-coupling-driven CDW mechanism in FeGe [28]. However, due to the extremely large supercell required for the incommensurate CDW phases, such as the $7 \times 7 \times 2$ supercell for $\mathbf{Q}_{\text{ICDW2}}$, further structural and energetic analyses could not be obtained within a reasonable computational time (see Sec. IX of the Supplemental Material [47]).

The strained FeGe lattice remains dynamically stable without imaginary phonon frequencies up to 4% strain. With strain higher than 4%, negative phonon bands develop in FeGe and persist at high temperatures (see Fig. S2 of the Supplemental Material [47]).

According to previous studies [28,46], strong electronic correlations, represented by the on-site Coulomb repulsion Hubbard U , play a crucial role in phonon instabilities. Therefore, we examine the impact of strong electronic correlations on the phonon spectra of FeGe under in-plane tensile strain

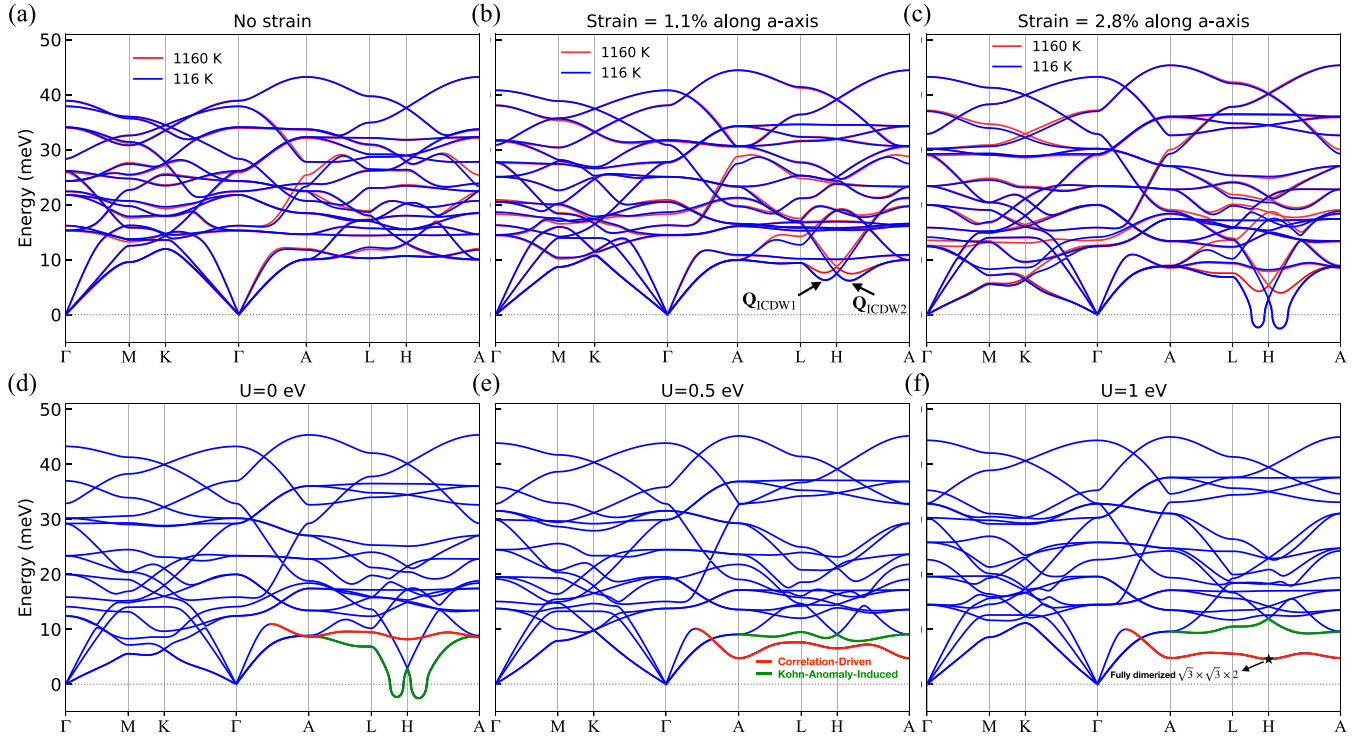


FIG. 2. Panels (a)–(c) show the phonon spectra under different levels of the *ab*-axis tensile strain. The red and blue lines represent simulations applying Fermi smearing temperatures with broadening corresponding to 1160 and 116 K, respectively. The positions of $\mathbf{Q}_{\text{ICDW1}} = (0.24, 0.38, 0.5)$ and $\mathbf{Q}_{\text{ICDW2}} = (0.28, 0.28, 0.5)$ are indicated by black arrows. Panels (d)–(f) present the phonon spectra calculated with different Hubbard U values: 0, 0.5, and 1 eV at a Fermi smearing temperature of 116 K and under 2.8% tensile strain along *ab* axis. The red and green lines highlight the phonon bands associated with electron correlation and Kohn anomaly, respectively. (f) The black star indicates the phonon mode corresponding to the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase.

of 2.8%, as shown in Figs. 2(d)–2(f). As the Hubbard U increases from 0 to 1 eV, both $\mathbf{Q}_{\text{ICDW1}}$ and $\mathbf{Q}_{\text{ICDW2}}$ phonon modes are gradually stabilized accordingly, indicating that enhanced electronic correlations suppress the strength of electron-phonon coupling due to the relatively localized electron picture.

Furthermore, with increasing Hubbard U , two pronounced phonon softenings emerge at the high-symmetry *H* and *A* points. By analyzing the soft phonon modes at these two points, we identified two distinct structural instabilities: a fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase [Fig. 1(e)] and a $1 \times 1 \times 2$ CDW phase (see Fig. S3 of the Supplemental Material [47]), respectively. In contrast to the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase observed in high-pressure experiments, the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase obtained from the *H*-point soft phonon mode exhibits large Ge-1 dimers formed at all Ge-1 sites, indicating a fully saturated dimerized state, as illustrated in Fig. 1(e). Regarding the $1 \times 1 \times 2$ CDW phase obtained from the *A*-point phonon mode, a preliminary total-energy assessment revealed that the corresponding structure is energetically unfavorable under tensile strain (see Fig. S3 of the Supplemental Material [47]); therefore, no further investigations were performed.

Our analysis of the phonon spectra reveals that under lateral tensile strain, FeGe exhibits both conventional electron-phonon-induced Kohn anomalies and unconventional correlation-driven phonon softening modes, suggesting

a competition between two distinct CDW mechanisms of fundamentally different origins.

To clarify the underlying mechanism of the strain-induced CDW phase transitions, we performed total-energy analyses of the possible CDW phases in laterally strained FeGe, including the pristine phase, the $2 \times 2 \times 2$ CDW phase [17,18], the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase [40,41], and the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase obtained from the softened phonon mode at the *H* point [Fig. 2(f)]. Figure 3(a) shows that the tensile strain induces a CDW phase transition from the $2 \times 2 \times 2$ phase to the $\sqrt{3} \times \sqrt{3} \times 2$ phase at about 0.6% strain. This CDW transition is similar to that observed in previous high-pressure experiments and DFT calculations [40,41]. As the strain increases to approximately 2.4%, a new type of CDW phase transition emerges—from the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase to the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase. Since FeGe is a moderately correlated electron system, inclusion of the Hubbard U is generally required in DFT total-energy calculations. At $U = 0.2$ eV, the strain required for the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase transition decreases to $\sim 0.2\%$ and that for the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase is reduced to slightly less than 1.8%, as illustrated in Fig. 3(b). From the total-energy results, only about 1.8% tensile strain along the *ab* axis is sufficient to induce both CDW phase transitions, suggesting a high feasibility for experimental verification. In addition, the effect of compressive in-plane strain on the CDW phases is also examined. As shown in

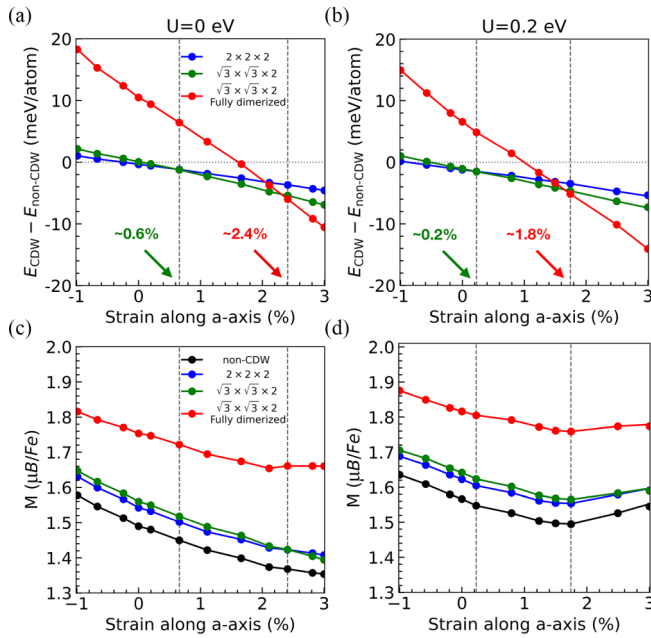


FIG. 3. Total energies and magnetic moments of FeGe CDW lattice structures under in-plane tensile strain. Panels (a) and (b) show the total energies per atom of three CDW phases with $U = 0$ and $U = 0.2$ eV, respectively, referenced to the total energy per atom of the pristine phase. The vertical gray dashed lines highlight the strains of the CDW phase transitions. Panels (c) and (d) show the average magnetic moments per Fe atom of the pristine phase and three CDW phases.

Fig. 3, when a small compressive strain (-1%) is applied, the total energies of all CDW phases increase to positive values, indicating that compressive strain suppresses CDW formation. Therefore, we do not pursue this direction further.

Since FeGe exhibits A-type AFM, each individual Fe kagome layer can be regarded as ferromagnetic. Therefore, the average magnetic moment per Fe atom within a single layer can be used as a measure of the magnetic strength. Figures 3(c) and 3(d) show the average magnetic moment within Fe Kagome layer under tensile strain without U and with $U = 0.2$ eV, respectively. In general, magnetic order in magnetic materials is monotonically suppressed under pressure or strain associated with enhanced orbital overlap [53,54]. In

strained FeGe, however, we observe an anomalous nonmonotonic evolution of magnetism with increasing strain in Figs. 3(c) and 3(d): The magnetic moment initially decreases and then increases at larger strain. Notably, the increase occurs only after the transition from the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase to the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase, indicating the distinct magnetic character of the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase. The microscopic origin of this anomalous magnetic enhancement in strained FeGe remains unclear, but it is likely related to the increased number of large Ge-1 dimers. Experimentally, when FeGe transitions from the pristine phase to the $2 \times 2 \times 2$ CDW phase [18], a slight enhancement of the magnetic moment is observed along with the formation of Ge-1 dimers. In our DFT calculations, the application of 1.8% tensile strain can induce fully dimerized CDW phase transition within the $\sqrt{3} \times \sqrt{3} \times 2$ supercell, leading to the formation of additional Ge-1 dimers and ultimately resulting in the energetically favorable fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase. As the number of Ge-1 dimers increases, the magnetic moment strengthens accordingly, suggesting a correlation between the formation of Ge-1 dimers and the enhancement of magnetism (see Sec. VI of the Supplemental Material [47]).

Finally, we present the electronic band structures of FeGe at zero strain and at 2.8% strain, and discuss the influence of electronic correlations by varying the Hubbard $U = 0$, 0.2, and 0.5 eV, as shown in Figs. 4(a)–4(c), respectively. The VHSs in the characteristic kagome band structure are considered to be one of the driving factors for the CDW in FeGe [17,18], as both ARPES measurements and DFT calculations show that the VHSs lie near the Fermi level, thereby promoting CDW instability. However, in both high-pressure experiments and DFT calculations on FeGe, the $2 \times 2 \times 2$ CDW phase and the $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase become more stabilized, while the VHSs move away from the Fermi level [40,41]. This observation suggests that the VHSs may not be the primary driving mechanism of the CDWs in FeGe. In the band structures of strained FeGe, we observe a behavior consistent with previous high-pressure studies: Under tensile strain, the VHS at the M point shifts away from the Fermi level. Moreover, as the Hubbard U increases, this shift of the VHS further away from the Fermi level becomes even more pronounced. These results indicate that the VHS is unlikely to be the primary driving mechanism of the CDWs in FeGe.

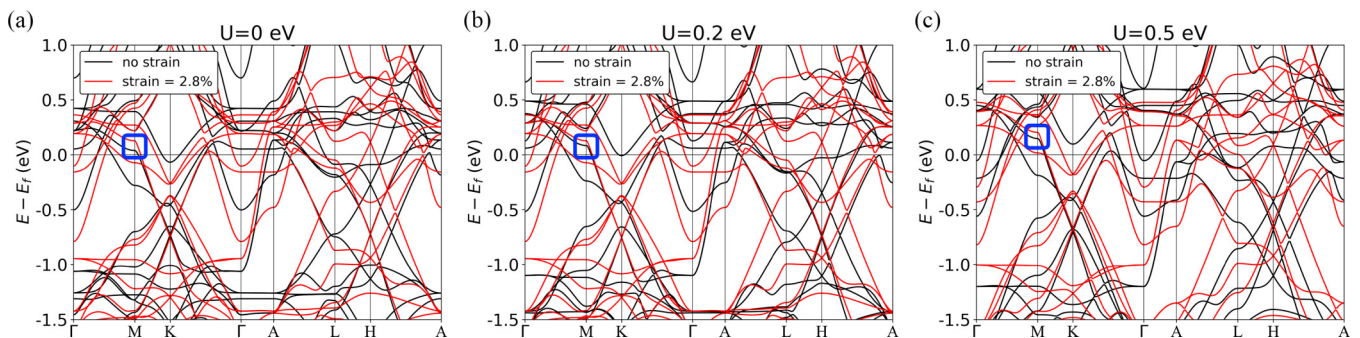


FIG. 4. (a)–(c) Band structures calculated with different Hubbard U values: 0, 0.2, and 0.5 eV, respectively. The black and red lines represent no strain and 2.8% strain, respectively. The blue boxes indicate the locations of the VHSs.

IV. CONCLUSION

In this work, we systematically investigated how in-plane tensile strain modulates CDW phases in the magnetic kagome metal FeGe. Our phonon band structure analyses reveal the emergence of two Kohn-anomaly-driven incommensurate CDWs, $\mathbf{Q}_{\text{ICDW1}}$ and $\mathbf{Q}_{\text{ICDW2}}$, together with a correlation-driven fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase. By comparing the total energies of the relevant CDW structures, we establish a clear strain-induced cascade of CDW transitions, $2 \times 2 \times 2 \rightarrow \sqrt{3} \times \sqrt{3} \times 2 \rightarrow$ fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$, highlighting the rich structural landscape that tensile strain can access. For instance, for the pressure-induced $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase transition, a pressure of approximately $P = 15$ GPa is required [40,41], corresponding to nearly 3% strain along the *ab* axis in our DFT simulations. In contrast, strain engineering requires only about 0.2% strain to induce the CDW phase transition. Furthermore, a moderate strain of approximately 1.8% can even stabilize a fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase. These results indicate that strain provides a much more experimentally accessible and efficient route for tuning CDW phases.

Moreover, the transition into the fully dimerized $\sqrt{3} \times \sqrt{3} \times 2$ CDW phase is accompanied by an anomalous increase of magnetism under tensile strain, deviating from the

conventional monotonic suppression typically expected in magnetic materials [53,54].

Overall, our findings demonstrate that strain engineering offers a powerful and experimentally accessible route to uncover and tailor the hierarchy of competing CDWs in magnetic kagome FeGe. The coexistence and competition between electron-phonon-driven incommensurate CDWs and correlation-driven dimerized CDWs position FeGe as a rare platform for probing strongly coupled spin-charge-lattice entanglement in kagome systems. These predictions provide concrete targets for future neutron, X-ray, and ARPES studies, and establish strained FeGe as a promising arena for realizing and controlling emergent orders in correlated topological materials.

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DATA AVAILABILITY

The data that support the findings of this study are available from the authors upon reasonable request.

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