

## Lattice dynamics study of electron-correlation-induced charge density wave in antiferromagnetic kagome metal FeGe

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Electron-correlation-driven phonon soft modes have been recently reported in the antiferromagnetic kagome FeGe compound and associated with the observed charge density wave (CDW). In this paper, we present a systematic investigation of the CDW origin in the context of the *ab initio* lattice dynamics study. Performing the group theory analysis of the aforementioned soft modes, we found that the stable structure has the Immm symmetry and can be achieved by shifts of Ge atoms. The occurrence of two soft modes induces the first-order phase transition, which leads to the CDW order. Additionally, we show that the final structure realizes a distorted honeycomb Ge lattice, as well as a nonflat kagome-like Fe net. For completeness, we present the electronic properties calculations. From the theoretical STM topography simulation, we indicate that the observed CDW occurs in the deformed honeycomb Ge sublattice.

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Kagome lattice materials attract significant attention due to their unique electronic properties [1], such as flat bands, van Hove singularities (VHSs) at the M point, and Dirac cone dispersion at the K point. From this, a wide range of exotic properties and behaviors emerge in the kagome lattice due to different degrees of electron filling [2–4]. For example, a strong correlation can induce magnetic order [5,6], while a VHS close to the Fermi level can lead to lattice instability and charge density wave (CDW) [7,8]. The kagome lattices can also exhibit topological properties [1,9–11] not only limited to the electronic structure [12–17]. Therefore, the kagome lattice materials provide an excellent platform to study new physical phenomena.

Recently, we have learned about several kagome lattice systems which exhibit interesting properties. Here, we can mention Weyl semimetal  $\text{Co}_3\text{Sn}_2\text{S}_2$ , with ferromagnetic Co kagome net [18–23]. Topological properties and the break of the time reversal symmetry lead to the intrinsic giant anomalous Hall effect [18,24,25], while hosting of the exotic Weyl fermions [19] induces the appearance of the Fermi arc [20]. Another example,  $\text{AV}_3\text{Sb}_5$  ( $A = \text{K}, \text{Rb}, \text{and Cs}$ ) with a vanadium kagome net displays the CDW with the Star of David (SoD) pattern below  $\sim 90$  K [26–28]. Moreover, below  $\sim 2$  K the coexistence of CDW and superconducting state is observed [10,29,30]. Such compounds can also exhibit an unconventional anomalous Hall effect [31,32]. Finally, other well-studied kagome systems, such as FeSn [33–36], CoSn [36–38],  $\text{Fe}_3\text{Sn}_2$  [39–41],  $\text{RTi}_3\text{Bi}_4$  ( $R = \text{Yb}, \text{Pr}, \text{and Nd}$ ) [42–44],  $\text{MMn}_6\text{Sn}_6$  ( $M = \text{Y}, \text{Er}, \text{Tb}$ ) [45–52], and  $\text{ScV}_6\text{Sn}_6$

[53,54], or  $\text{AV}_6\text{Sb}_6$  ( $A = \text{K}, \text{Rb}, \text{Cs}, \text{or Gd}$ ) [11,55–58] can also be mentioned.

In this Letter, we focus on FeGe, in which CDW was recently discovered [59,60]. FeGe exhibits an antiferromagnetic (AFM) order below 410 K [61–67]. At room temperature, the Fe atoms are ferromagnetically coupled with the kagome sublattice plane and antiferromagnetically coupled between kagome sublattices, i.e., along  $c$  [so-called A-AFM order, see Fig. 1(d)]. At lower temperatures, a tilt of the Fe magnetic moments from the  $c$  axis was reported. The CDW phase is reported below 100 K [59]. The coexistence of these two ordered phases provides a great opportunity to study the interplay between them [59,68]. The scanning tunneling microscopy (STM) of the surface charge distribution uncovers the  $2 \times 2$  pattern [59,69,70].

In this context, it is important to recognize correctly the origin of the CDW. For example, in the case of vanadium kagome net systems ( $\text{AV}_3\text{Sb}_5$ ) the CDW is associated with imaginary soft modes at the M and L points [71–74], which induce the structural phase transition [72,75]. These soft modes lead to a stable structure with the  $C2/m$  [72] or  $Fmmm$  [73] symmetry. The phonon spectrum of FeGe, calculated without electron correlations, is similar to the other CoSn-like compounds [76], and no imaginary soft modes are observed. However, the introduction of the correlations leads to the softening of some optical phonons along the L-H direction [70,77,78]. Such soft modes generate the Ge-dimerization and were recognized as a source of CDW [79]. Nevertheless, a more thorough dynamical study of the CDW formation mechanism has not yet been performed. Here, using the *ab initio* techniques, we derive a critical value of the on-site Coulomb interaction, which induces imaginary soft modes in the phonon spectrum.

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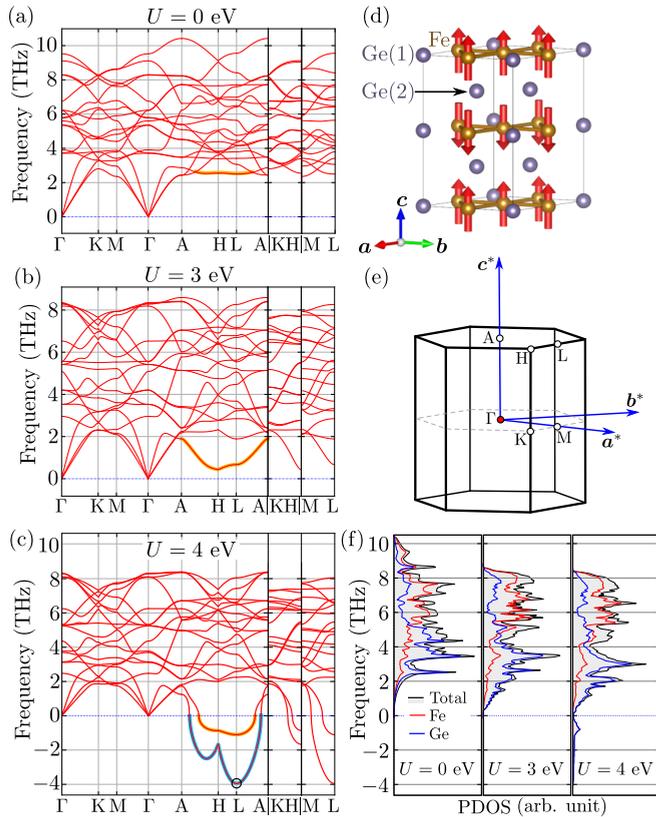


FIG. 1. (a)-(c) The effect of the local Coulomb interaction on the phonon dispersion curves along high symmetry directions for FeGe with the P6/mmm symmetry. Results for a different Hubbard  $U$  parameter (as labeled). (d) Magnetic unit cell of FeGe with the P6/mmm symmetry in the presence of the A-AFM order, and its Brillouin zone (e). (f) The phonon DOS as a function of the local Coulomb interaction value.

Detailed analysis of the symmetry of these soft modes allow us to find a stable low-symmetry structure of FeGe.

**Computational techniques.** The first-principle's density functional theory (DFT) calculations were performed using the projector augmented-wave (PAW) potentials [80] implemented in Vienna *Ab initio* Simulation Package (VASP) [81–83]. For the exchange-correlation energy, the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) parametrization was used [84]. The energy cutoff for the plane-wave expansion was set to 350 eV. We introduced the correlation effect on Fe 3d orbitals using the DFT +  $U$  scheme proposed by Dudarev *et al.* [85]. It is worth mentioning that the use of the Liechtenstein *et al.* approach [86] changed results only quantitatively [see Fig. S1 and Fig. S2 in the Supplemental Material (SM) [87]].

The optimization of the lattice constants and atomic positions in the presence of the spin-orbit coupling (SOC) was performed for magnetic unit cells (with the collinear A-AFM order). The structures were optimized with different  $\mathbf{k}$ -grids generated using the Monkhorst-Pack scheme [88], depending on the investigated symmetry. The initial structure with the P6/mmm symmetry was optimized using  $8 \times 8 \times 5$   $\mathbf{k}$ -point grid. Structures with the Ibam and Immm symmetries were optimized with  $15 \times 8 \times 8$   $\mathbf{k}$ -point grids. As a convergence

criterion of the optimization loop, we took the energy change below  $10^{-6}$  eV and  $10^{-8}$  eV for ionic and electronic degrees of freedom, respectively. The symmetry of the structures after optimization was analyzed with FINDSYM [89] and SPGLIB [90], while momentum space analysis was performed within SEEK-PATH [91].

Dynamic properties were calculated using the direct Parlinski-Li-Kawazoe method [92], implemented in the PHONOPY package [93,94]. Within this method, the interatomic force constants (IFC) are calculated from the Hellmann-Feynman (HF) forces acting upon all atoms after displacements of individual atoms inside the supercell. We performed these calculations using the supercell with the shape corresponding to  $2 \times 1 \times 2$  magnetic unit cells with the Ibam and Immm symmetries (approximately cubic shaped, containing 24 formula units). During these calculations, a reduced  $5 \times 5 \times 5$   $\mathbf{k}$ -grid was used.

For the final crystal structure, the STM topographies were simulated within the Tersoff-Hamann approach [95] for the slab containing four FeGe layers (with fixed atomic positions) separated by  $\sim 10$  Å of vacuum.

**Dynamical properties and system stability.** Let us start with a discussion of the lattice dynamics for the initial structure with the P6/mmm symmetry, in the presence of different values of Coulomb interaction on Fe  $d$  orbitals (Fig. 1). In the absence of the correlations ( $U = 0$  eV), none of the phonon dispersion curves show any noticeable softening nor imaginary values [see Fig. 1(a)] [76]. The introduction of Hubbard  $U$  causes the softening of the lowest phonon mode along the H-L direction [70,77,78]. This is clearly visible when we compare that phonon branch for  $U = 0$  eV and  $U = 3$  eV [cf. Fig. 1(a) and 1(b), where the soft mode is marked with an orange background]. However, further increase of  $U$  (e.g., to 4 eV) leads to the emergence of imaginary soft modes [presented as negative frequencies in Fig. 1(c)]. As we can see, there is some critical value of the Hubbard parameter ( $U_c$ ) for which the soft modes become imaginary. At this higher  $U$  value, there are two imaginary soft branches [marked with orange and blue in Fig. 1(c)]. The branch marked with an orange background corresponds to the soft mode visible for  $U < U_c$  in Fig. 1(b).

In Fig. 1(f) the phonon density of states spectra were compared for various values of the Hubbard  $U$  parameter. Increasing the local Coulomb potential (from 0 eV to 4 eV) causes an enhancement of both the magnetic moments of the iron atoms (from  $1.53 \mu_B$  to  $2.96 \mu_B$ ) and the crystal cell volume (by about 12%). However, it is worth emphasizing that phonon softening is not connected with volume extension but only with correlation effects, which we verified by changing volume and  $U$  separately. What is more surprising, the increasing in value of  $U$  on Fe results in a softening of phonon modes associated mainly with the vibrations of Ge atoms: Ge(1) perpendicular and Ge(2) parallel to the Fe kagome layers (marked with orange and blue in Fig. 1(c), respectively). We should briefly discuss the magnitude of  $U$  for Fe  $d$  orbitals. The effective Hubbard  $U$  parameter of 4 eV was used for Fe-based compounds, mainly iron oxides such as FeO [96], Fe<sub>2</sub>O<sub>3</sub> [96], Fe<sub>3</sub>O<sub>4</sub> [97], or Fe<sub>2</sub>SiO<sub>4</sub> [97]. In some cases a larger effective  $U$  is necessary (e.g., for iron-bearing sphalerite [98]). For metals, due to the screening effects, the

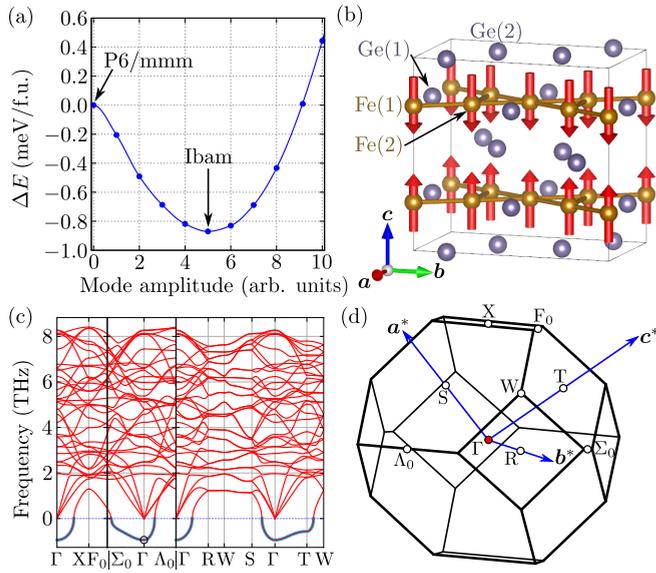


FIG. 2. (a) The soft mode amplitude dependence of the system's energy for the distorted structure induced by the soft mode at the L point of the P6/mmm structure. The zero of energy scale is set at the energy of the initial P6/mmm structure. The optimized system with the lowest energy has the Ibam symmetry and magnetic unit cell, presented in panel (b). In (c), the phonon dispersion curves for FeGe with the Ibam symmetry along high symmetry directions of the Brillouin zone are presented following the scheme displayed in (d).

$U$  parameter is usually smaller [99]. The comparison of Fe magnetic moments with the experimental value of  $1.7 \mu_B$  also indicates a smaller value of  $U$  in FeGe [100]. Here, we assumed  $U = 4$  eV to demonstrate the existence of the soft mode with the frequency approaching zero and becoming imaginary. Such a gimmick allowed for the study of a structure with lower symmetry. In reality, as the diffraction studies on FeGe showed, the phase transition to the CDW phase has the 1st-order character [59,77]. In such a case, the soft mode does not need to go to zero frequency to trigger the structural transformation and, therefore, a real value of  $U$  is smaller than 4 eV. Nevertheless, as we mentioned earlier, for  $U > U_c$  the phonon dispersion curves show imaginary soft modes. Since structural changes are defined by the polarization vector of the soft mode, the resulting space group symmetry is independent of  $U$ .

Let us now analyze displacements induced by the lowest energy soft mode occurring at  $L = (0, 1/2, 1/2)$ . Condensation of such a mode enforces doubling of the P6/mmm primitive unit cell along the  $b$  and  $c$  directions. Additionally, freezing of displacements induced by its polarization vector lowers system energy because of the imaginary value of the soft mode frequency. In fact, the system's energy as a function of the displacement amplitude directly shows the existence of a structure with the lower energy [Fig. 2(a)]. This displaced and more stable structure will be the "base" of our further analysis.

The structure with the P6/mmm symmetry (space group No. 191) possesses the lattice parameters  $a = b = 5.163$  Å and  $c = 4.251$  Å. The atoms are located at three nonequivalent Wyckoff positions: (3f) Fe (1/2, 0, 0), (1a) Ge(1) (0, 0, 0), and (2d) Ge(2) (1/3, 2/3, 1/2). The Fe atoms form an ideal

kagome net, decorated by Ge(1) in the same plane. The Ge(2) atoms form the honeycomb lattice, located between the kagome layers. The AFM magnetic order leads to doubling of the unit cell along the  $c$  direction [see Fig. 1(d)], i.e., the magnetic unit cell contains 6 formula units. The L-point imaginary mode leads mainly to the displacement of Ge(2) atoms (along the  $a + b$  direction of the P6/mmm structure) by about  $\pm 0.06$  Å [see Fig. 3(a) in the SM [87]]. We should also mention that the Fe atoms still form a kagome-like net with two different distances between atoms: Fe(1)–Fe(2) and Fe(2)–Fe(2) equal to 2.5860 Å and 2.5809 Å, respectively. The optimized structure has the Ibam symmetry (space group No. 72), with lattice constants  $a = 5.158$  Å,  $b = 8.956$  Å, and  $c = 8.501$  Å, and four nonequivalent Wyckoff positions: (4a) Fe(1) (0, 0, 1/4), (8e) Fe(2) (1/4, 1/4, 1/4), (4b) Ge(1) (1/2, 0, 1/4), and (8j) Ge(2) (0.5142, 0.6654, 0). Just like before, Ge(1) atoms decorate the kagome net, while Ge(2) atoms form the deformed honeycomb-like lattice. The magnetic unit cell corresponds to the conventional cell and is presented in Fig. 2(b). The ground state energy of the system with the magnetic moment on Fe atoms along  $c$  and tilted from  $c$  axis are close to each other.

The phonon dispersion curves for the optimized Ibam structure are presented in Fig. 2(c). As we can see, the phonon spectrum still contains imaginary soft modes (marked with blue lines) and the most predominant soft mode occurs at the  $\Gamma$  point. In that case, the structure can be stabilized by shifts of atoms, mostly Ge(1), that do not modify the size of the unit cell. As a result, we can apply the same strategy as before to find the final crystal structure.

The dependence of the system's energy on the displacement amplitude of the polarization vector of the soft mode at the  $\Gamma$  point for the Ibam structure is presented in Fig. 3(a). The most important displacement is associated with the shift of the Ge(1) atoms along the  $c$  direction [see Fig. S3(b) in the SM [87]], which is in agreement with the previous theoretical studies [79], where the large dimerization of Ge(1) sites was studied without breaking the P6/mmm symmetry. The soft mode of Ibam structure leads to the Immm symmetry (space group No. 71). After optimization, the total energy decreases and lattice parameters read  $a = 5.158$  Å,  $b = 8.956$  Å, and  $c = 8.501$  Å. The atoms are located in the Wyckoff positions: (4j) Fe(1) (1/2, 0, 0.2353), (8k) Fe(2) (1/4, 1/4, 1/4), (4i) Ge(1) (0, 0, 0.8462), (4h) Ge(2) (0, 0.3063, 1/2), and (4g) Ge(3) (0, 0.3515, 0). Similarly, the energies of the system with Fe magnetic moments along the  $c$  axis and tilted from the  $c$  direction are comparable. In this structure, the Ge(1) atoms are shifted from their initial positions by  $\pm 0.82$  Å along the  $c$  direction [in practice, the distance between Ge(1) atoms decreases from 4.06 Å (P6/mmm) to 2.61 Å (Immm), what corresponds to effective shifting of 0.725 Å]. That large modification of the atomic position leads indirectly to large deformation of the Fe kagome-like net and the Ge honeycomb sublattice [see Figs. 3(c) and 3(d)]. The kagome-like lattice is not flat, while the deviation from the plane is around 0.13 Å. The distances between Fe atoms within the kagome-like net are 2.5791 Å and 2.5839 Å for Fe(2)–Fe(2) and Fe(2)–Fe(3), respectively. Similarly, the new distances between atoms in the deformed honeycomb sublattice are 2.94 Å and 2.66 Å for Ge(2)–Ge(3) and Ge(3)–Ge(3), respectively.

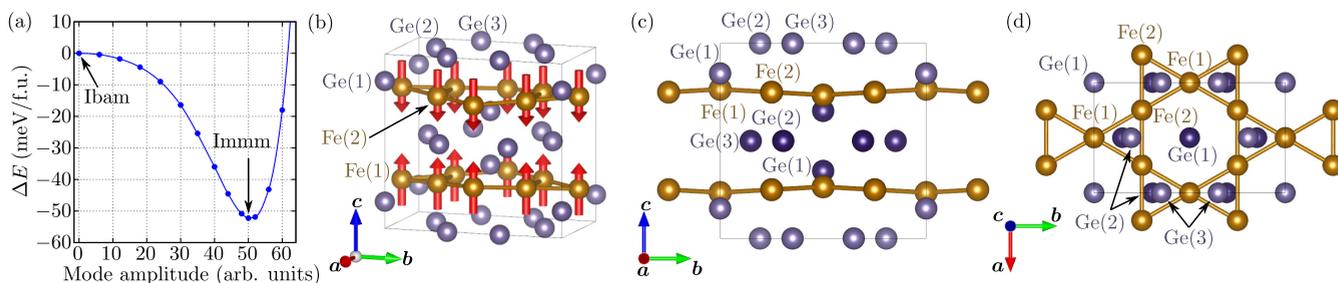


FIG. 3. (a) The soft mode amplitude dependence of the system's energy for the structure induced by the soft mode of the Ibam structure at the  $\Gamma$  point. Energy changes are given relative to the ground-state energy of the Ibam structure. Mode amplitude, expressed as displacement of Ge(1) atoms:  $u_{\text{Ge}} \approx 0.8 \text{ \AA}$ . The system reaches the lowest energy for the Immm symmetry, with the magnetic unit cell presented in (b). The front and top view of the crystal with the Immm symmetry is presented in (c) and (d) panels, respectively.

The phonon dispersion curves and phonon density of states for the final structure are presented in Fig. 4. As we can see, the structure with the Immm symmetry is dynamically stable. The vibrations associated with Fe atoms are mostly realized by the phonon modes in the higher frequency range, while the lowest modes correspond to the vibrations of Ge. Acoustic branches around the  $\Gamma$  point show well-visible linearity. The first nearly flat bands within the Brillouin zone are located above 2 THz (8.27 meV). Furthermore, a dense complex band structure is visible around 5 THz (20.68 meV), while phonon branches with the highest frequencies are around 9 THz (37.22 meV). These frequency ranges are in excellent agreement with the experimentally observed phonon spectrum [68].

From the above analysis it is clear that the final stable structure arises from the condensation of two soft modes, the first at the L point of P6/mmm structure and the second at the  $\Gamma$  point of the intermediate Ibam symmetry. The structural transformation involving two soft modes (two order parameters) leads to the first order phase transition, in which the crystal structure changes discontinuously at the critical temperature. This scenario agrees with the experimental observation of the CDW phase in FeGe [59,77]. As we demonstrated, the soft mode frequency strongly depends on  $U$ , which modifies the Fe  $d$  states, and thus influences the interatomic forces.

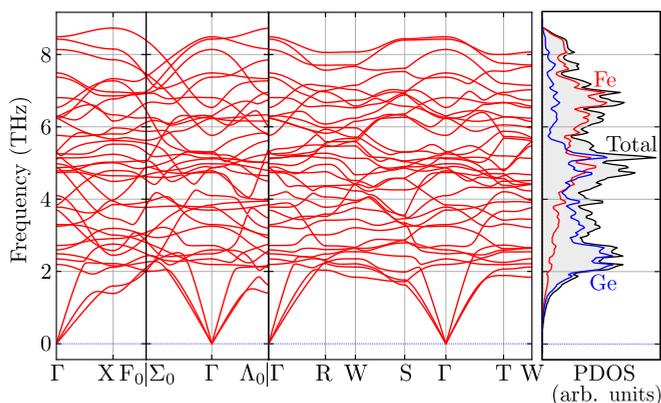


FIG. 4. The phonon dispersion curves along high symmetry directions and phonon density of states for FeGe with the Immm symmetry. The symbols of the high symmetry points are the same as in Fig. 2(d).

Moreover, analyzing the IFC changes introduced by  $U$ , we noticed that the strongest effect is observed for the diagonal component  $zz$  of the on-site Ge force constant matrix. With the increasing  $U$ , this force constant decreases significantly, leading to a softening of the phonon modes. It shows that the electron-phonon coupling plays an important role in the mechanism of structural deformation and the CDW formation.

Crystal symmetry breaking, which leads to the CDW phase, is well-visible in the Raman spectroscopy measurements [101]. The structural transition at  $T_{\text{CDW}}$  gives rise to the appearance of new Raman active modes in the higher frequency range for  $T < T_{\text{CDW}}$ . Indeed, both P6/mmm and Immm symmetries are characterized with a different number of the Raman active modes (see Table S1 in the SM [87]). The calculated frequency of the  $A_g$  mode in the low-temperature tetragonal phase very well corresponds to the measured value [101]. Unfortunately, the Raman spectroscopy does not provide clear information about the symmetry of the final crystal structure. However, the atomic displacements should modify the x-ray diffraction pattern (XRD). The significant difference between the XRD for both structures can be found in the simulated XRD pattern (see Fig. S4 in the SM [87]). Consequently, the XRD measurement at low temperatures can be used to confirm the predicted symmetry.

*Electronic properties.* The electronic band structures for the P6/mmm and Immm magnetic unit cells (see Fig. S5 in the SM [87]) possess several similarities. This suggests that the electronic spectra observed within angle-resolved photoemission spectroscopy (ARPES) measurements should be similar for the system both before and after the transition to the CDW phase. The same behavior is also observed in vanadium-based kagome systems  $AV_3Sb_5$  [102–105], where modification of the electronic ARPES spectra is mostly connected with a transition to the CDW phase.

In the case of P6/mmm structure, all Fe atoms carry a magnetic moment of  $2.96 \mu_B$ . An additional magnetic moment is also induced on the Ge(1) atoms ( $0.165 \mu_B$ ). As we mentioned earlier, the transition from the P6/mmm to Immm phase leads to modification of the magnetic moments. The deformation of the kagome net causes a small increase of the Fe(1) magnetic moment ( $3.00 \mu_B$ ), while the Fe(2) magnetic moment remains unchanged ( $2.96 \mu_B$ ). Similarly, the shift of Ge(1) in the Immm structure, with respect to its position in the initial P6/mmm symmetry, leads to a small decrease of the magnetic moment on Ge(1) ( $0.125 \mu_B$ ). Additionally,

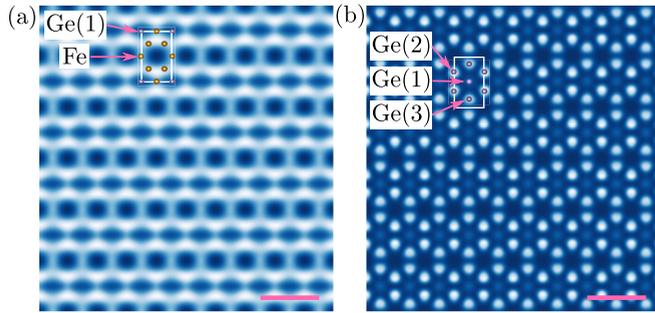


FIG. 5. Theoretically obtained STM topography of FeGe with the Immm symmetry, calculated  $\sim 1 \text{ \AA}$  above the surface. Results for termination on Fe kagome-like net (a), and deformed Ge honeycomb lattice (b). Inset presents the relative position and unit cell for the (001) surface. Scale bar,  $\sim 1 \text{ nm}$ .

the Ge(1) magnetic moment has an opposite direction to the nearest Fe kagome-like net.

For the Immm structure obtained here, we can simulate the STM topography for two different (001) surface terminations (see Fig. 5). The results presented are based on DFT slab calculations, while the STM topography comes from the  $E_F \pm 0.1 \text{ eV}$  energy window. In Figs. 5(a) and 5(b) we present the theoretically obtained STM topography for the FeGe terminated on the Fe kagome-like net and the deformed Ge honeycomb lattice, respectively. Comparison to the experimentally reported STM pattern [59] suggests that FeGe has termination on the deformed Ge honeycomb lattice. In the case of theoretically obtained results, both topographies are similar to the CDW stripe order. However, the Fourier transform of the experimental STM topography shows that the CDW peaks have a non-equal intensity [59]. In fact, one of the CDW peaks

is much stronger than the other, which can suggest a stripe type of the CDW order. Moreover, from a theoretical point of view, the  $2 \times 2$  CDW order in the P6/mmm structure due to the shift of Ge(1) out of the Fe kagome layer corresponds to the stripe order in the Immm structure, as presented in Fig. 5(b).

*Summary.* Starting from the initial P6/mmm structure, which contains an ideal Fe kagome net, we found that there exists a critical value of the Hubbard  $U$  parameter ( $\sim 3.5 \text{ eV}$ ), for which the softened phonon mode becomes imaginary. From analysis of the most predominant imaginary soft branch at the L point, we found a new structure with the Immm symmetry. This structure comes from P6/mmm due to the shift of Ge atoms within the Fe kagome net layer. However, the lattice dynamics of the Immm structure reveals that it is also unstable with soft mode at the  $\Gamma$  point. In this case, the displacement introduced by this soft mode associated with the shift of Ge atoms in a direction perpendicular to the Fe kagome net leads to a stable Immm structure. Condensation of both modes leads to the first-order structural phase transition, which is, in turn, responsible for the formation of the CDW. It is also worth noting that the occurrence of the first-order phase transition in FeGe is confirmed by experiments.

For completeness, we also performed calculations for the slab structure with the Immm symmetry to generate STM images for the Fe-kagome-like and Ge-deformed honeycomb surface terminations. The calculated STM topographies indicate the existence of charge ordering. The observed CDW phase is associated with a deformed Ge honeycomb-like lattice.

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