

The Effects of Pressure on the Structural, Electronic, and Lattice Dynamical Properties of FeSe Superconductor

Hong-Yan Lu · Ni-Na Wang · Meng-Jun Wei ·
San Chen · Yang Yang · Ding-Fu Shao ·
Wen-Jian Lu

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Abstract Motivated by the experimental huge enhancement of the superconducting transition temperature T_c in FeSe superconductor under high pressure, we perform first-principles calculations of the evolutions of structural, electronic, and lattice dynamical properties of FeSe at varying hydrostatic pressures up to 8 GPa. The pressure response is anisotropic with a larger compressibility along c -axis. At ambient pressure, Fermi surface nesting between hole and electron pockets induces spin density wave (SDW) order at the vector $(\pi, \pi, 0)$ with a collinear antiferromagnetic structure. With the increase of pressure, the Fermi surface nesting is reduced, and therefore the SDW is suppressed, which could not enhance superconductivity based on the spin-fluctuation scenario. For the phonon dispersion, the bands have blue-shift except for the modes around 100 cm^{-1} , indicating hardening of the vibration modes in a wide frequency range. Furthermore, the electron–phonon coupling constant and the corresponding T_c by McMillan equation are calculated. However, there is no obvious enhancement of T_c under pressure, which further rules out the conventional phonon-mediated superconductivity of FeSe. Maybe the local magnetic moment plays an important role for the superconductivity and enhancement of T_c under pressure.

H.-Y. Lu (✉) · N.-N. Wang · M.-J. Wei · S. Chen
School of Physics and Electronic Information, Huaibei Normal University, Huaibei 235000, China
e-mail: luhongyan2006@sohu.com

Y. Yang
College of Physics and Electronic Engineering, Zhengzhou University of Light Industry, Zhengzhou 450002, China

D.-F. Shao · W.-J. Lu
Key Laboratory of Materials Physics, Institute of Solid State Physics, Chinese Academy of Sciences, Hefei 230031, China

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1 Introduction

In the recent years, iron-based superconductors have received tremendous attention since the discovery of superconductivity in F-doped layered LaOFeAs with transition temperature T_c of 26 K [1]. Then, some new types of iron-based superconductors have been found, including the 111-type [2], 122-type [3,4], and 11-type [5] in addition to the original 1111-type [1,6,7]. Among them, FeSe [5], which is a 11-type superconductor with T_c of 8 K, has attracted great attention due to its simple atom composition, simple lattice structure, and the absence of toxic As atom. Under ambient conditions, it has tetragonal PbO-type structure with space group $P4/nmm$ and consists of square Fe-atom plane with Se atoms forming distorted tetrahedra around Fe. On the superconducting mechanism, theoretical results based on linear response theory show that the electron–phonon coupling constant λ is smaller than 0.2 and the corresponding T_c is even no more than 1 K [8,9], ruling out the conventional phonon-mediated superconductivity. However, the large Fe isotope effect exponent in FeSe ($\alpha_{Fe} = 0.81$) [10] indicates that the phonons originating from Fe vibrations are important. On the other hand, ^{77}Se NMR experimental results suggest that FeSe superconductor is on the verge of spin density wave (SDW) ordering and antiferromagnetic (AFM) spin fluctuations are strongly enhanced near T_c [11]. Therefore, there may be a positive link between AFM spin fluctuations and the superconducting mechanism of FeSe.

It is well known that the pressure is a clean and effective way to change the structure and modify the physical properties of materials. Pressure-induced superconductivity is of particular interest, from which we can extract the structure characteristics that superconductivity favors. The effects of pressure on the structure and superconductivity of FeSe have been experimentally studied [12–16]. Under applied pressure, the unit-cell volume and lattice parameters decrease, and it is more compressible along c axis than along a or b axes [13,14,16]. Mizuguchi et al. found a huge enhancement of the superconducting transition temperature T_c under pressure, with the onset temperature as high as 27 K at 1.48 GPa and the huge pressure coefficient of 9.1 K/GPa [12]. Besides, Garbarino et al. studied the structure and superconducting properties of FeSe under applied pressures up to 26 GPa. A phase transition was observed from the tetragonal to an orthorhombic symmetry at 12 GPa. T_c increases with the increase of pressure and can even reach 34 K at 22 GPa in the orthorhombic phase [13]. Similar enhancement of T_c was found by Miyoshi et al. [15], while Margadonna et al. found a nonmonotonic T_c (P) behavior with a maximum T_c of 37 K around the pressure 7 GPa [16]. It is meaningful to investigate how pressure influences the electronic structure and the lattice dynamics properties of FeSe from the ab-initio point of view. This is the topic of the present paper.

In this paper, using first-principles calculations, we study the evolutions of structural, electronic, and lattice dynamical properties of FeSe at varying hydrostatic pressures up to 8 GPa. For the electronic structure, the band structure, density of states (DOS), Fermi surface (FS), and the nesting effect of FS are calculated from 0 to 8 GPa.

While for the lattice dynamical properties, we study the phonon dispersion, phonon DOS, as well as the electron–phonon coupling constant and the corresponding T_c using McMillan equation in the same range of pressure.

2 Computational Details

The calculations are performed in a plane-wave pseudopotential representation through the Quantum-Espresso (QE) program [17]. We adopt ultrasoft pseudopotentials to model the electron–ion interactions and the generalized gradient approximation (GGA) with Perdew–Burke–Ernzerhof parametrization [18] for the exchange correlation potentials. The energy convergence is checked with respect to the cutoff energy and k-point sampling. The cutoffs for wave functions and charge density are 70 and 700 Ry, respectively. The electronic integration is performed over a $8 \times 8 \times 8$ k-point mesh. Within the framework of the density functional perturbation theory (DFPT) [19] in the linear response method [20],¹ we calculate the lattice dynamics and the electron–phonon coupling constant. The dynamical matrices are calculated on a $4 \times 4 \times 4$ q-point grid. A denser $16 \times 16 \times 16$ k-point grid is used for evaluating an accurate electron–phonon interaction matrix. Besides, we use a $30 \times 30 \times 30$ k-point grid to calculate the FS, nesting function, and Lindhard function.

To obtain the structures under different pressures from 0 GPa to 8 GPa, the initial lattice parameters of FeSe in our calculations are based on the experimental value under ambient conditions: $a = b = 3.765$ Å, $c = 5.518$ Å [5]. Note that our calculations are based on the nonmagnetic order, and there are two Fe atoms and two Se atoms in the unit cell. We fully optimize the structural parameters of FeSe with increasing hydrostatic pressure by simultaneously varying the cell volume and cell parameters. It should be noted that there is no structural phase transition in the studied range of pressure. After that, we calculate the electronic and lattice dynamical properties of FeSe based on the optimized structure.

3 Results and Analysis

We now present and discuss the numerical results. Firstly, we show the optimized structure, including the lattice parameters a , c , the ratio c/a , the internal coordinate of Se, i.e., Z_{Se} , and the unit-cell volume V with the increase of pressure from 0 to 8 GPa as shown in Fig. 1. From Fig. 1a, we can see that the lattice parameter a decreases from 3.68 to 3.60 Å and c decreases from 6.02 to 5.02 Å. The ratio c/a also decreases, with the value changing from 1.63 to 1.39 as shown in Fig. 1b. This means that the pressure response on the structure is anisotropic with a larger compressibility along c -axis. From Fig. 1c, we find that the internal coordinate of Se increases monotonously

¹ In the linear response method, the displacement of atoms can be viewed as a perturbation. Response functions such as total charge density and force induced on the atoms are linear with the perturbation. In the framework of DFPT [19], the total energy after perturbation can be obtained, while the force constants matrices are the second differential of the total energy. Then, the dynamical matrices, which correlate with phonon properties, can be obtained by Fourier transformation of force constants matrices.

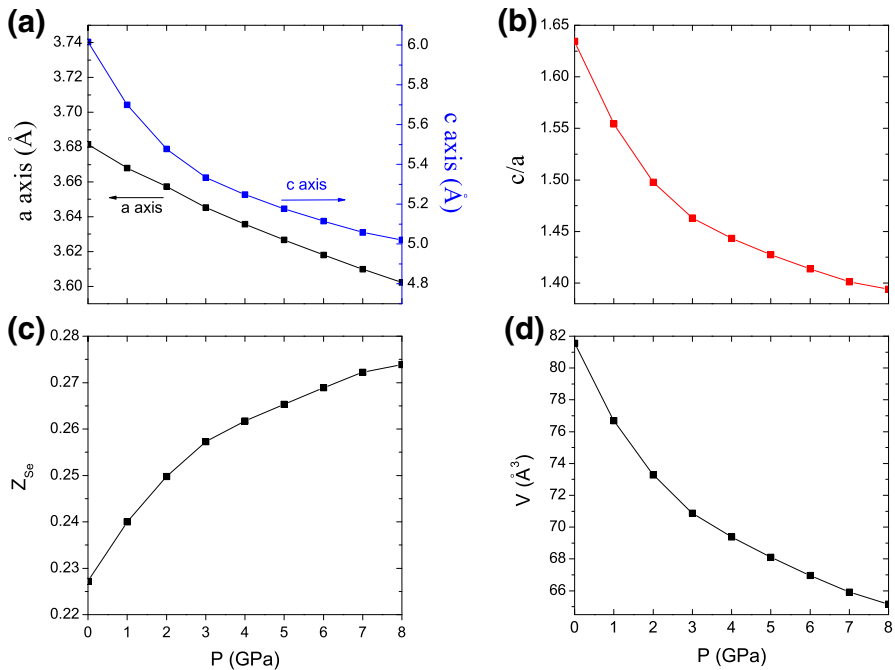


Fig. 1 The optimized lattice parameters a , c (a), the ratio c/a (b), the internal coordinate of Se, i.e., Z_{Se} (c), and the unit-cell volume V (d) of FeSe as a function of the applied pressure (Color figure online)

with the increase of applied pressure. Figure 1d shows that the unit-cell volume V decreases from 81.6 to 65.2 Å³. These results are very close to the experimental data [13, 14].

Based on the optimized structural parameters, we calculate the electronic, lattice dynamical properties of FeSe under the applied pressure. The calculated electronic band structures of FeSe along high-symmetry lines at $P = 0, 4$, and 8 GPa are shown in Fig. 2. At 0 GPa, crossing the Fermi energy, there are two electronic-like FS sheets around M-A line and three hole-like FS sheets around Γ -Z line. This can be clearly seen from the FS sheets shown in Fig. 3a. It is found that there are two distorted electronic cylinders around M-A line and three hole-like sheets around Γ -Z line: one inner near closed pocket and two outer cylinders, well consistent with previous theoretical result [21, 22]. To see clearly the effect of pressure on the band structure, we put the 0 and 4 GPa results in one figure (Fig. 2a), while the 4 and 8 GPa results in another figure (Fig. 2b). By comparing them, it can be seen that with the increase of pressure, most parts of the bands above the Fermi energy move to higher energy, while most of those below the Fermi energy move to lower energy, leading to a broader electronic bandwidth. This is understandable that the applied pressure reduces the distance between Fe and Se atoms. Therefore, the electronic orbits of adjacent atoms become more overlapped, which would lead to broader bandwidth. For the FS under pressure, we draw the result at $P = 4$ GPa in Fig. 3b. Both the electron and hole FS sheets are distorted. We also

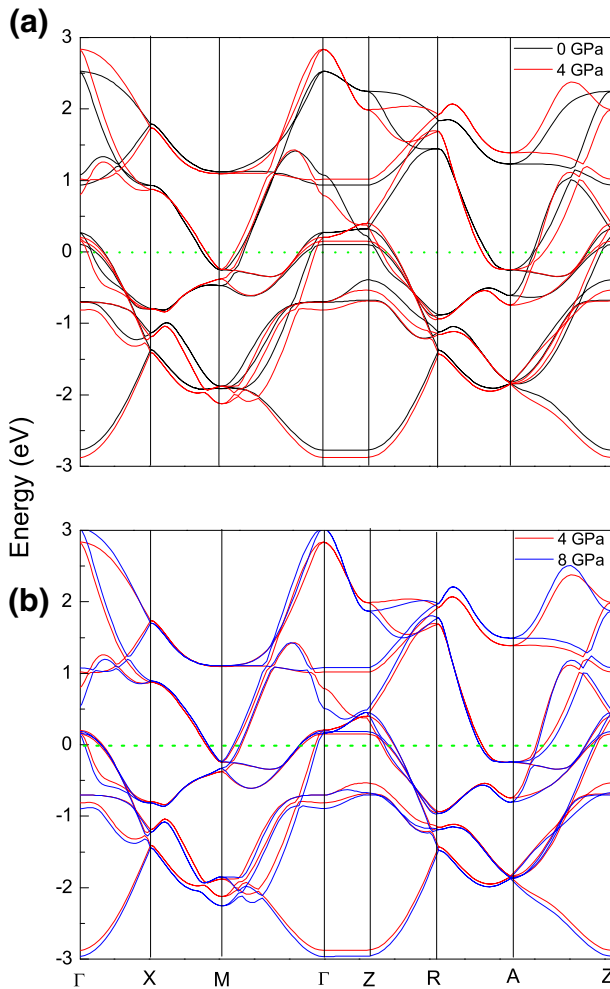


Fig. 2 The electronic band structures of FeSe along high-symmetry lines at $P = 0$ GPa, 4 GPa (a), and $P = 4$ GPa, 8 GPa (b). The Fermi energy is set to be zero (Color figure online)

calculate the FS at $P = 8$ GPa (not shown here), and the FS sheets of the five bands through the Fermi level are further distorted.

To quantitatively estimate the effect of pressure on the nesting of FS, we firstly determine the nesting vector by calculating the nesting function, which could be obtained by [23]

$$\xi(q) = \frac{1}{N} \sum_k \delta(\varepsilon_k - E_F) \delta(\varepsilon_{k+q} - E_F). \quad (1)$$

Here N is the number of k points in the sum, ε_k and ε_{k+q} are the eigenvalues obtained by the first-principles calculations, and E_F is the Fermi energy. Then, to estimate the nesting effect, we calculate the Lindhard function by

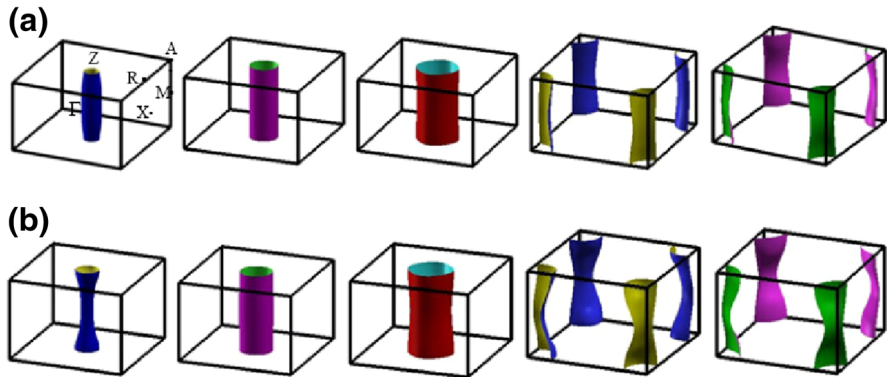


Fig. 3 The FS sheets of the five bands through the Fermi level at **a** 0 GPa and **b** 4 GPa (Color figure online)

$$\chi(q) = -\frac{1}{N} \sum_k \frac{f(\varepsilon_k - E_F) - f(\varepsilon_{k+q} - E_F)}{\varepsilon_k - \varepsilon_{k+q}}, \quad (2)$$

where f is the Fermi-Dirac distribution function. The calculated nesting function and Lindhard function for FS in $k_z = 0$ plane at 0 GPa and 4 GPa can be seen in Fig. 4. From Fig. 4a, we can see the nesting function at 0 GPa is peaked at the M point $(\pi, \pi, 0)$. This is the nesting vector, by shifting of which the electronic FSs around M and the hole FSs around Γ can largely overlap. The Lindhard function also shows a peak at $(\pi, \pi, 0)$ as shown in Fig. 4b, indicating a significant nesting effect. Due to this fact, SDW or spin fluctuation may be the mechanism of superconductivity in FeSe, which is supported by the NMR experiment [11]. Considering that there are two Fe atoms in the unit cell of nonmagnetic FeSe, the calculated $(\pi, \pi, 0)$ nesting just corresponds to the $(\pi, 0, 0)$ nesting in the 1-Fe sublattice, i.e., the collinear AFM order. This is well consistent with previous theoretical result that collinear AFM order has the lowest energy among all the possible orders in FeSe [24]. This order has also been theoretically predicted in the undoped binary Fe chalcogenide superconductor FeTe [25]. For the parent compound of Fe–As-based materials, the collinear AFM order has also been verified as the ground state by neutron scattering [26] and has been reproduced by model simulation [27]. However, there are other orders such as bi-collinear AFM in Fe_{1+x}Te [25], block AFM in $\text{R}_{1-x}\text{Fe}_{2-y}\text{Se}_2$ [28] and BaFe_2Se_3 [29], and pair-checkerboard order in monolayer FeSe thin film [30,31], which have also been theoretically predicted in the iron-based superconductors family.

Then, we discuss the effect of pressure on FS nesting. At the applied pressure of 4 GPa, Fig. 4c shows that the peak of nesting function is decreased and changed to a cylindrical plateau centered at M point. Meanwhile, the peak of the Lindhard function in Fig. 4d also decreases compared with the 0 GPa result, indicating that the nesting effect is reduced. We also calculate the nesting function and Lindhard function for FS in $k_z = \pi/c$ plane at 0 GPa and 4 GPa, and the suppression of nesting effect under pressure is also found. Besides, the two functions at 8 GPa are also calculated. It is found that the intensities around $(\pi, \pi, 0)$ for both functions are nearly reduced to zero, suggesting that SDW disappears. The increase of applied pressure

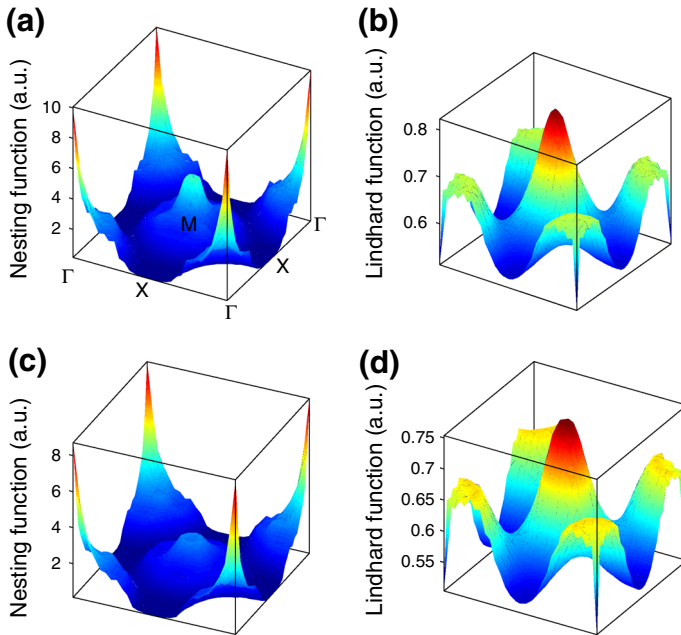


Fig. 4 **a** and **b** are the calculated nesting function and Lindhard function for FS in $k_z = 0$ plane at 0 GPa, respectively. **c** and **d** are those for 4 GPa case (Color figure online)

gradually destroys the SDW state. However, experiments show a great enhancement of T_c with applied pressure [12, 13, 15]. Therefore, the pure spin-fluctuation scenario for the superconductivity could not explain this phenomenon.

We also calculate the total DOS and the projected DOS to Fe-3d and Se-4p orbitals at 0, 4, and 8 GPa (not shown here). The states at the Fermi level are predominantly of Fe-3d character with a slightly hybridization with Se-4p orbital, no matter at ambient pressure or at applied pressures. Of particular importance is the DOS at the Fermi energy, i.e., $N(E_F)$, which determines many physical properties of superconducting FeSe. Therefore, we draw the pressure dependence of $N(E_F)$ as shown in Fig. 5. We can see $N(E_F)$ increases from 2.82 states/eV at 0 GPa to a maximum value of 3.02 states/eV at 7 GPa, and then decreases to 3.01 states/eV at 8 GPa. This mainly originates from the increase of the Fermi energy under applied pressure. The behavior of $N(E_F)$ may correlate with the enhancement of T_c under relatively low pressure [12, 13, 15] and the specific nonmonotonic $T_c(P)$ behavior with the maximum T_c around the pressure 7 GPa [16].

Next, we show and discuss the effects of pressure on the lattice dynamical properties of superconducting FeSe. The calculated phonon dispersion curves at 0, 4, and 8 GPa as well as the corresponding phonon DOS (PDOS) and atom-projected PDOS are plotted in Figs. 6 and 7, respectively. From Fig. 6a and b, we can see that nearly all bands move upwards, or have a blue-shift with the increase of pressure, showing pronounced hardening of the original vibration modes. Only some modes around 100 cm^{-1} have red-shift, indicating softening of the original vibration modes. From Fig.

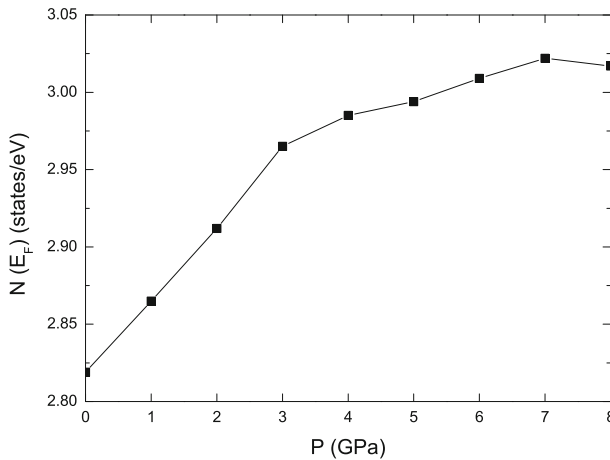


Fig. 5 Pressure dependence of the DOS at Fermi energy (Color figure online)

7a, we can see that, at 0 GPa, the vibration modes in high-frequency range ($\omega > 230 \text{ cm}^{-1}$) are mainly contributed by Fe atoms, while those in the middle-frequency range ($100 \text{ cm}^{-1} < \omega < 230 \text{ cm}^{-1}$) are mainly contributed by Se atoms. This is because Se atom has larger mass than Fe atom. In the low-frequency range ($\omega < 100 \text{ cm}^{-1}$), Fe atom and Se atom contribute comparatively to the total PDOS. By comparing Fig. 7a, b and c, it is found that the PDOS peaks move to higher frequencies with the increase of pressure. Another evident feature is that the vibration modes of Fe atoms in the middle-frequency range are greatly enhanced, reaching a fair contribution to the total PDOS with those of Se atoms.

Furthermore, based on the BCS theory, we check whether the superconducting transition temperature T_c is enhanced under applied pressure as reported in the experiments. Within the framework of DFPT [19] in the linear response method [20] as implemented in the QE program [17], we calculate the electron–phonon coupling constant λ and the logarithmic average frequency ω_{log} for pressures from 0 GPa to 8 GPa. We find that the maximum λ is about 0.184 at $P = 2 \text{ GPa}$, which is little strengthened compared with the value $\lambda = 0.133$ at $P = 0 \text{ GPa}$. Then we calculate T_c using the Allen-Dynes modified McMillan equation [32],

$$T_c = \frac{\omega_{log}}{1.2} \exp \left[\frac{-1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right], \quad (3)$$

where μ^* is Coulomb pseudopotential and usually takes a value around 0.1. However, the obtained maximum value of T_c is only 0.214 K at $P = 2 \text{ GPa}$ even if μ^* is set to zero. This is even less than the reported T_c of 8 K at ambient pressure, not to mention the enhanced T_c at applied pressures. Therefore, our calculations once more rule out the conventional phonon-mediated superconductivity in FeSe, consistent with previous result under ambient pressure [8,9].

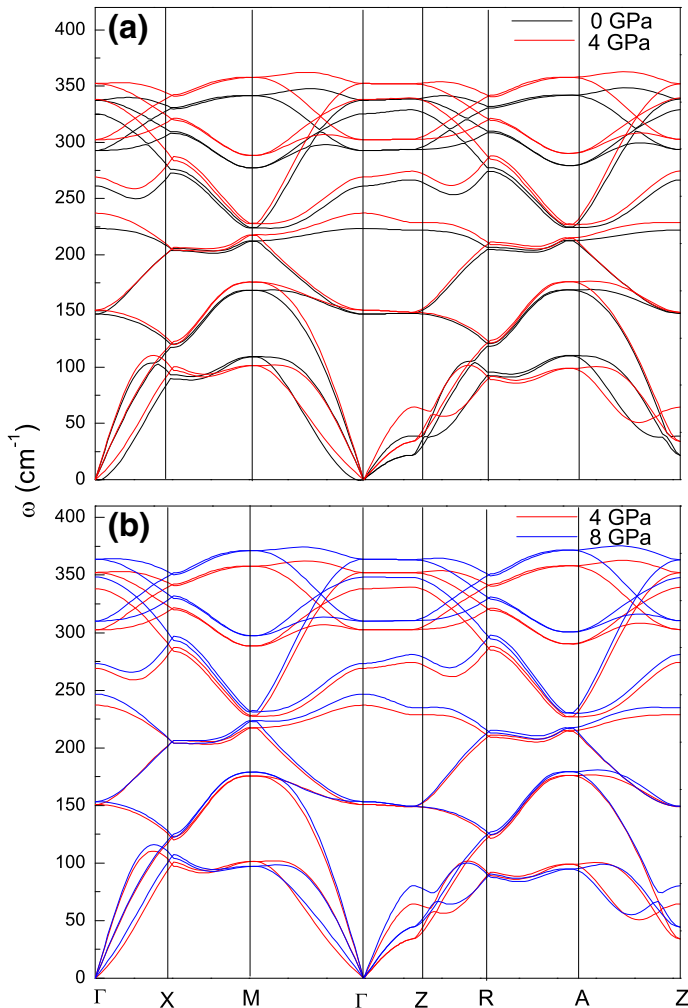
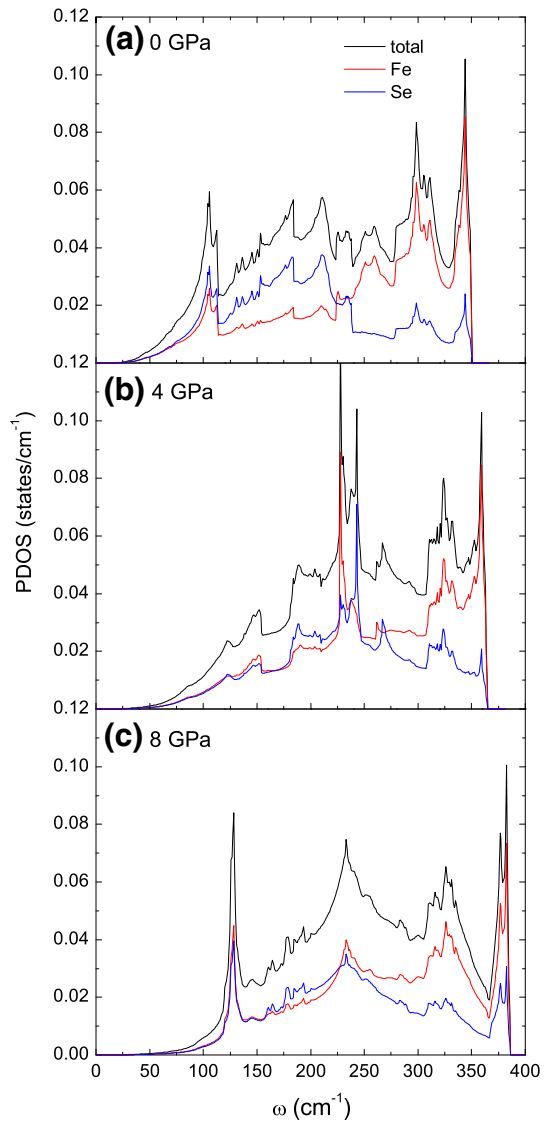


Fig. 6 The phonon dispersion curves of FeSe along high-symmetry lines at $P = 0$ GPa, 4 GPa (**a**) and $P = 4$ GPa, 8 GPa (**b**) (Color figure online)

4 Discussion and Summary

Based on our above nonmagnetic order calculations, we make some discussions. It has been shown that the non-spin-resolved electron–phonon pairing mechanism could neither account for the T_c at ambient pressure, nor explain the great enhancement of T_c under pressure. In comparison, from first-principles studies based on the spin-resolved electron-phonon pairing, no matter in the checkerboard or the striped spin pattern, at ambient pressure, T_c has a little increase compared with the non-spin-resolved case, but still far from the experimental value [9,33]. Therefore, the phonon-mediated superconductivity may be ruled out, but the effect of phonons could not

Fig. 7 The calculated total phonon DOS and atom-projected phonon DOS of FeSe at $P = 0$ GPa (a), 4 GPa (b), and 8 GPa (c) (Color figure online)



be ignored. From our above calculations of the dynamical properties, the frequencies of all optical phonon modes in the Brillouin zone center increase with the applied pressure. Especially, the vibrations of Fe atoms are greatly enhanced, consistent with the calculations based on the checkerboard AFM order [34].

On the magnetic origin of iron-based superconductors, there are mainly two contradictory views. One is based on the itinerant electron picture, in which superconductivity is mediated by the FS nesting or the AFM spin fluctuation [25, 35]. For $\text{LaFeAsO}_{1-x}\text{F}_x$, this picture can result in a sign reversal of the order parameter between hole and electron pockets [35], while the other is based on the local magnetic moment interactions

and can be described by the J_1 - J_2 model [36–38]. Nevertheless, the inelastic neutron scattering experiments in SrFe_2As_2 [39] and CaFe_2As_2 [40] show that the magnetic excitations can be described by the spin waves based on local-moment Heisenberg model, suggesting a mixing of local and itinerant magnetism in the parent compounds of iron arsenide superconductors. Based on our calculated results, there is obvious nesting effect or spin fluctuation in FeSe at ambient pressure. However, with the increase of applied pressure, the nesting effect is suppressed and gradually disappears. Therefore, the pure itinerant electron picture could not explain the great enhancement of T_c under pressure. It is speculated that the local magnetic moment may be an important factor for the superconductivity and enhancement of T_c under pressure.

To summarize, the evolutions of structural, electronic, and lattice dynamical properties of FeSe at varying hydrostatic pressures up to 8 GPa have been studied based on first-principles calculations. The evolution of structure accounts nicely with the experimental results. For the electronic structure, the electronic bandwidth is broadened and the density of states at the Fermi energy is nonmonotonic, i.e., firstly increases and then decreases with a maximum at 7 GPa. At ambient pressure, FS nesting between hole and electron pockets induces SDW order with a collinear AFM structure. The FS nesting is reduced under pressure, which suppresses SDW and could not enhance superconductivity based on the spin-fluctuation picture. For the phonon dispersion, the optical phonon modes show obvious hardening. Furthermore, the calculated value of T_c under pressure based on BCS theory is far less than the experimental result, further ruling out the conventional phonon-mediated superconductivity of FeSe. Therefore, we speculated that the local magnetic moment plays an important role for the superconductivity and enhancement of T_c of FeSe under pressure.

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