Ab initio prediction of pressure-induced structural phase transition of superconducting FeSe

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Abstract

External pressure driven phase transitions of FeSe are predicted using ab initio calculations. The calculations reveal that \( \alpha \)-FeSe makes transitions to NiAs-type, MnP-type, and CsCl-type FeSe. Transitions from NiAs-type to MnP-type and CsCl-type FeSe are also predicted. MnP-type FeSe is also found to be able to transform to CsCl-type FeSe, which is easier from \( \alpha \)-FeSe than the transition to MnP-type FeSe, but comparable to the transition from NiAs-type FeSe. The calculated electronic structures show that all phases of FeSe are metallic, but the ionic interaction between Fe–Se bonds becomes stronger and the covalent interaction becomes weaker when the structural phase transition occurs from \( \alpha \)-FeSe to the other phases of FeSe. The experimentally observed decrease in \( T_c \) of superconducting \( \alpha \)-FeSe at high pressure may be due to a structural/magnetic instability, which exists at high pressure. The results suggest an increase of the \( T_c \) of \( \alpha \)-FeSe if such phase transitions are frustrated by suitable methods. (Some figures may appear in colour only in the online journal)

1. Introduction

FeSe has been studied for its magnetic properties [1–3] and shows a phase transition from \( \alpha \)-FeSe to \( \beta \)-FeSe (tetragonal to hexagonal) as the growth temperature is increased [2]. Interest in \( \alpha \)-FeSe has grown since Hu et al [4] observed superconductivity with a \( T_c \sim 8 \) K because it is structurally related to the newly existing investigations of FeAs superconductors [5] and subsequently the \( T_c \) was increased by the application of pressure [6, 7] and doping [8]. External pressure up to 2.2 GPa enhances both the spin fluctuations and the \( T_c \) in \( \alpha \)-FeSe [9]; however a large external pressure further decreases \( T_c \) [6].

Experimental results show that tetragonal FeSe undergoes a structural transition to a hexagonal phase [10] and at 12.5 GPa to an orthorhombic phase [11]. More recently, Medvedev et al [6] reported the increase of \( T_c \) from 8.5 to 36.7 K under an applied pressure of 8.9 GPa and also showed a phase transition from tetragonal to NiAs-type hexagonal at 12 GPa. Compared with the FeAs superconductors [5], which also show a structural phase transition from tetragonal to orthorhombic [12, 13], \( \alpha \)-FeSe has not only the same planar sublattices, but also displays structural and magnetic instabilities [14].

Albeit FeSe shows structural transitions, it is not clear how the electronic structure responds to external pressure, and what the transition path of FeSe should be. It is then invaluable to study FeSe in different crystallographic environments to observe the effects of structural changes upon changing the atomic volume or applying pressure. Thus, because of its relative chemical simplicity compared with FeAs superconductors, FeSe provides a unique opportunity to study the interplay of the structure, magnetism, and superconductivity. Therefore, determination of the structural and magnetic phase transitions in FeSe is essential for understanding their electronic
properties. To our knowledge, no systematic study has been performed to explore the mechanism of the structural phase transitions in stoichiometric FeSe. We show that there are structural and magnetic phase transitions at high pressure. Such phase transitions also affect the magnetic, electronic, and bonding properties of FeSe; these are considered as an indirect clue for improving the $T_c$ of FeSe.

This paper is organized as follows. We describe the computational models and methods which are used to investigate the structural phase transitions of FeSe in section 2. In section 3 we discuss our calculated results, i.e., structural phase transition, magnetism, and electronic structures of FeSe. The results and discussion are summarized in section 4.

2. Computation models and methods

To search for the structural phase transition of FeSe, we considered different types of crystal structure, i.e., anti-PbO, commonly known as $\alpha$-FeSe, as well as NiAs-, MnP-, CsCl-, and CuAu-type FeSe (see figure 1). These structures are related with each other, e.g., MnP-type FeSe can be considered as a deformed NiAs-type FeSe, changing the local hexagonal symmetry around the Fe atoms in the NiAs-type phase to tetrahedral results in the $\alpha$-FeSe phase. The detailed structural relationships will be discussed in section 3.

$Ab\ initio$ calculations were performed using the total-energy all-electron full-potential linearized augmented plane-wave (FLAPW) method [15] in the QMD-FLAPW package [16] based on both the local spin density approximation (LSDA) [17] and the generalized gradient approximation (GGA) [18]. Integrations inside the Brillouin zone (BZ) were performed by the improved tetrahedron method [19] over a $15 \times 15 \times 15$ mesh within the three dimensional (3D) BZ and with an energy cutoff at $4.10 (2\pi/a)$, where $a$ is the lattice parameter of each calculation. A $16.36 (2\pi/a)$ star-function cutoff was used for depicting the charge and potential in the interstitial regions. Lattice harmonics with $l \leq 8$ were employed to expand the charge density, potential, and wavefunctions inside each muffin-tin (MT) sphere of radius 2.2 au for Fe and 1.9 au for Se. The convergence of the computation parameters was checked carefully [20].

All core electrons were treated fully relativistically and valence states were calculated scalar relativistically, i.e., without spin–orbit coupling [21]. The explicit orthogonalization (XO) procedure was employed to ensure the orthogonality between the semicore and valence states with the spill-out of each MT sphere semicore charge being superposed [22]. Self-consistency was assumed when the difference between input and output charge densities became less than $1.0 \times 10^{-4}$ electrons au$^{-3}$.

The calculated total energy–volume ($E-V$) data were fitted to the Birch–Murnaghan equation of state [23] which enabled us to calculate the enthalpy $H = E + pV$, where $E$ is the internal energy, $p$ is the external pressure, and $V$...
The calculated total energy in units of eV/f.u. as a function of lattice volume (Å³) for α-FeSe and (a) NiAs-, (b) MnP-, (c) CsCl-, and (d) CuAu-type FeSe. The total energy was measured with respect to the total energy of the α-FeSe equilibrium volume. The filled circles (squares) show the total energy in the NM (FM) state. The red, black, cyan, green, and blue colors represent α-FeSe, NiAs-, MnP-, CsCl-, and CuAu-type FeSe, respectively. (e) shows the $E-V$ curve of all the structures in the volume interval 20–35 Å³.

Table 1. Structural parameters of FeSe. The final column shows the optimized volume $V$ (in units of Å³) per formula unit.

| Type      | Atom | Atomic positions | $u$ | $v$ | $V$   |
|-----------|------|------------------|-----|-----|-------|
| α-FeSe    | Fe(2a)| 0 0 0; $\frac{1}{3}$ $\frac{1}{3}$ 0 | —   | —   | 39.370|
|           | Se(2c)| $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$; 0 0 $\bar{u}$ | 0.243| —   | —     |
| NiAs-type | Fe(2a)| 0 0 0; 0 0 $\frac{1}{2}$ | —   | —   | 33.640|
|           | Se(2b)| $\frac{1}{3}$ $\frac{1}{3}$ $\frac{1}{2}$; $\frac{2}{3}$ $\frac{2}{3}$ $\bar{u}$ | 0.250| —   | —     |
| CuAu-type | Fe(2a)| 0 0 0; $\frac{1}{2}$ $\frac{1}{2}$ 0 | —   | —   | 31.890|
|           | Se(2b)| $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$; 0 $\frac{1}{2}$ $\frac{1}{2}$ | —   | —   | —     |
| MnP-type  | Fe(4c)| $(0 v\frac{1}{2}, \frac{1}{2}; \frac{1}{2} - u, v + \frac{1}{2}, \frac{1}{2})$ | 0.200| 0.005| 29.000|
|           | Se(4c)| $(0 v\frac{1}{2}, \frac{1}{2}; \frac{1}{2} - u, v + \frac{1}{2}, \frac{1}{2})$ | 0.570| 0.190| —     |
| CsCl-type | Fe    | 0 0 0             | —   | —   | 28.370|
|           | Se    | $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ | —   | —   | —     |

is the volume of the system. All calculations were carried out for nonmagnetic (NM) and ferromagnetic (FM) states at different volumes. The optimized lattice parameters of α-FeSe were calculated to be $a = 3.747$ (3.701) Å, $c/a = 1.474$ (1.505), and volume/atom ratio = 19.685 (19.078) Å³ with the GGA (LSDA) results which are comparable to the recent experimental values [11]. The calculated internal coordinates and the formula unit (f.u.) volumes of the considered crystals at individual equilibria are summarized in table 1. We carefully checked that the physics of these systems does not depend sensitively on the details of the internal parameter values.

3. Results and discussion

3.1. Structural phase transition

In figure 2, one can see that α-FeSe is the most stable structure and under sufficient volume contraction (external pressure) α-FeSe becomes unfavorable compared to the other phases of FeSe. Around the equilibrium volume of α-FeSe all other phases are in metastable states by an energy barrier per f.u. of order 1.0 eV. As we compress the unit cell volume, α-FeSe goes to a higher energy state and NiAs-type FeSe becomes a stabilized phase. NM α-FeSe starts to cross...
Figure 3. The calculated enthalpy in units of Ryd as a function of pressure (GPa) for (a) $\alpha$-FeSe $\rightarrow$ NiAs-type, (b) $\alpha$-FeSe $\rightarrow$ MnP-type, (c) $\alpha$-FeSe $\rightarrow$ CsCl-type, (d) NiAs-type $\rightarrow$ CsCl-type, (e) NiAs-type $\rightarrow$ MnP-type, and (f) MnP-type $\rightarrow$ CsCl-type FeSe. The red, black, cyan, and green colors represent $\alpha$-FeSe, NiAs-type, MnP-type, and CsCl-type FeSe respectively. The dotted lines represent the NM states.

FM NiAs-type FeSe at a volume of $\sim$30.74 $\text{Å}^3$. Further compression transits $\alpha$-FeSe to the NM NiAs-type phase at 30.19 $\text{Å}^3$, but before crossing the NM NiAs-type FeSe phase, $\alpha$-FeSe crosses the energy curve of MnP-type FeSe. Hence, a slight compression deforms NiAs-type FeSe to MnP-type FeSe, where the hexagonal symmetry is broken and can be viewed as a distorted NiAs structure. We can also see that NM $\alpha$-FeSe begins to overcome FM MnP-type FeSe at about 30.33 $\text{Å}^3$ and NM MnP-type FeSe at about 29.86 $\text{Å}^3$.

NiAs-type FeSe can be transformed to CsCl-type FeSe if we push the Se atom to the center of the unit cell and simultaneously deform the $a$ and $b$ axes of the hexagonal lattice to a cubic lattice under a large external pressure, to break the bonds between the Fe and Se atoms in the hexagonal structure to make new bonds in the cubic structure. In other words, tetragonal $\alpha$-FeSe can be thought of as a distorted CsCl-type FeSe with an elongated $c$ axis. Hence, one can naturally expect a transition to CsCl-type FeSe at corresponding high pressure. On the other hand, MnP-type FeSe is a distorted structure where phase transition to CsCl-type FeSe will require a larger pressure as compared to NiAs-type FeSe. Although CuAu-type FeSe lies much higher in energy, extrapolating $\alpha$-FeSe to a small volume region tells us that $\alpha$-FeSe can enter into a metastable region at 27.80 $\text{Å}^3$ and CuAu-type FeSe may become a stable structure. However, the common tangent does not pass through both curves which makes the $\alpha$-FeSe to CuAu-type FeSe transition difficult. We must note that figure 2 gives an indication of the structural phase transitions of $\alpha$-FeSe under pressure, and the volumes discussed above are the critical volumes at which $\alpha$-FeSe crosses the binding curves of the other phases, e.g. NiAs-type FeSe.

The above discussion reveals the relative structural stability of $\alpha$-FeSe. However, to have a complete understanding of the phase transition of $\alpha$-FeSe, we calculated the transition pressures. The transition pressures ($p_t$) from $\alpha$-FeSe to the other structures, e.g., NiAs-type FeSe, can be obtained either
Table 2. Calculated structural transition pressures (in units of GPa) for FeSe. The available experimental data are taken from [11, 6].

| Transition        | Theory | Experiment |
|-------------------|--------|------------|
| α-FeSe→ NiAs-type | 17.50  | 12.0       |
| MnP-type          | 17.70  | 12.5       |
| CsCl-type         | 20.45  | —          |
| NiAs-type→ MnP-type| 21     | —          |
| CsCl-type         | 42     | —          |
| MnP-type→ CsCl-type| 60     | —          |

from the slope of the common tangent of both $E-V$ curves in figure 2 or from the usual condition of equal enthalpies, i.e., the pressure $p_t$ at which the enthalpies $H$ of α-FeSe and NiAs-type FeSe are the same. We follow the latter approach, since it is well known that the thermodynamic stable phase at some given pressure and zero temperature is the one with the minimum enthalpy [24]. At $p_t$, two phases have the same enthalpy, and then the transition pressure is determined by equating the enthalpies of the two phases of FeSe. Note that this is a standard procedure to calculate the transition pressure of materials [25–27]. To see the possible phase transitions, figure 3 shows the calculated enthalpy curves of α-FeSe, NiAs-, MnP-, CsCl-, and CuAu-type FeSe, respectively.

Following the above procedure, the transition pressures of FeSe are calculated and the results are summarized in table 2. The GGA (LSDA) $p_t$ of α-FeSe to NiAs-type FeSe is calculated to be $\sim 17.5$ (13.0) GPa, whereas the $p_t$ of α-FeSe to MnP-type FeSe is $\sim 17.70$ (13.05) GPa; these values are in agreement with recent experimental reports [6, 11]. It is clear that a slight external pressure deforms the hexagonal structure to the orthorhomic one. The experimental reports state that the structural phase transition from α-FeSe to MnP-type requires $\sim 0.5$ GPa more extra pressure than the transition to NiAs-type [6, 11]. Our calculations follow the same trend and the GGA (LSDA) results demonstrate that $\sim 0.20$ (0.05) GPa extra pressure than for NiAs-type is required for MnP-type FeSe. We also calculated the transition pressure of α-FeSe to CsCl-type FeSe which is $\sim 20.45$ GPa. Therefore, our calculations reveal that α-FeSe makes transitions to NiAs-type FeSe, MnP-type FeSe, and CsCl-type FeSe at high pressure irrespective of the magnetic structures. The predictions are in excellent agreement with recent experiments [2, 6, 11]. Table 2 also shows that there is a possibility of a phase transition from NiAs-type to CsCl-type FeSe at $\sim 42$ GPa. We can see that it is easier for α-FeSe to make the transition to NiAs- and then to MnP-type FeSe. However, a large external pressure of $\sim 60$ GPa is required for the MnP-type to CsCl-type FeSe phase transition. Further recent experimental observations found CsCl-type FeS [28], which is isoelectronic to FeSe, at high pressure and this supports the expectation of CsCl-type FeSe [29].

3.2. Magnetism

The calculated magnetic moments per Fe atom ($\mu_{Fe}$) are shown in figure 4. We did not find any magnetism in α-FeSe in the whole volume range, which is in agreement with recent first-principles calculations [30] and experiment [2]. The steps in $\mu_{Fe}$ of NiAs-type FeSe indicate that the magnetism of FeSe is sensitive to volume compression and expansion. Below the volume of 22 Å$^3$, NiAs-type FeSe has zero magnetic moment and the onset of magnetization can be seen for volumes greater than 22 Å$^3$; the small step in $\mu_{Fe}$ is due to the onset of magnetization. Once the magnetization develops, $\mu_{Fe}$ increases slightly and has a constant slope in the volume region 23–25 Å$^3$; this is the region where MnP-type FeSe is more stable in energy than NiAs-type FeSe. The step in $\mu_{Fe}$ occurs at $\sim 31$ Å$^3$, because near this volume hexagonal FeSe is more stable in energy than tetragonal FeSe. Interestingly, similar steps in $\mu_{Fe}$ can also be seen for MnP-type FeSe, where the onset of magnetization shifts to a higher volume region as compared with NiAs-type FeSe, i.e., the onset of magnetization starts at $\sim 25$ Å$^3$, exactly at the volume where FM MnP-type enters into FM NiAs-type FeSe. Then $\mu_{Fe}$ increases with increasing lattice volume and a change in slope can be seen around the volume region where α-FeSe crosses the energy curve of MnP-type FeSe. CuAu-type FeSe has zero $\mu_{Fe}$ for volumes $\leq$ 22 Å$^3$ and $\mu_{Fe}$ monotonically increases with the lattice volume. CsCl-type FeSe is more interesting due to its nonzero $\mu_{Fe}$ in the whole region of volume, and this may indicate that even if all the phases of FeSe become NM, CsCl-type FeSe retains its magnetic structure in an unconventional manner [29].

3.3. Electronic structures

The phase transitions described are understood by comparing the electronic structures in terms of the density of states (DOS). The calculated total and atom-projected DOSs in the FM states are shown in figure 5. The total DOS of α-FeSe shows metallic behavior which is in agreement with recent photoemission and transport measurements [1].
Figure 5. Total and atom-projected DOSs in the FM states of (a) α-FeSe, (b) NiAs-, (c) MnP-, (d) CsCl-, and (e) CuAu-type FeSe at their equilibrium lattice volumes. The red, blue, and green lines represent the Fe t$_{2g}$-, Fe e$_g$- and Se p-states, respectively, whereas the black lines in the bottom panels represent the total DOS. The Se p-states are multiplied by a factor of 10 and the Fermi levels ($E_F$) are set to zero. The total DOS is given per formula unit for comparison purposes.

exchange splitting is absent in α-FeSe and the Se p-states lie well below the Fermi energy ($E_F$). The Se p-states are hybridized with the Fe d-states and this hybridization is strong at a lower energy, $\sim -4.0$ eV. The strong peak near $E_F$ is formed mainly from the Fe e$_g$-states, and the Fe t$_{2g}$-states are more delocalized in energy and extend over a wide range of energy. The DOS shows that $E_F$ is dominated by the Fe d-states, which was also found in recent experimental results on α-FeSe [31] and the FeAs superconductor [32]. One can also see a pseudogap in the electronic structure of α-FeSe which was also found in previous calculations [33] and in the FeAs based superconductor [34]. This reveals that the electronic structure of α-FeSe is essentially similar to those of FeAs based superconductors.

The NiAs-type FeSe DOS in figure 5(b) shows a metallic property and now there is an exchange splitting between the majority and minority spins, which was absent in α-FeSe. Therefore, the structural phase transition is accompanied by a magnetic phase transition. Simultaneously, the Fe local symmetry is also changed from tetrahedral to octahedral. The Se p-states extend to lower energies and strongly hybridize mainly with the Fe t$_{2g}$-states. Furthermore, now there is no pseudogap in the majority spins, but it exists in the minority spin states. The peak at $\sim -2.0$ eV is contributed by the Fe t$_{2g}$-states. This switch of e$_g$- to t$_{2g}$-states is due to the change of local symmetry. Once the local symmetry of the Fe atom is changed to hexagonal (octahedral), further breaking of hexagonal symmetry will not have much affect on the electronic structure, as seen in the MnP-type FeSe DOS in figure 5(c). The electronic structure is identical to that of NiAs-type FeSe except for some minor changes around $E_F$ in the majority and minority spins. In the majority spins, $E_F$ lies in the valley; in the case of minority spins, the splitting between the t$_{2g}$- and e$_g$-states at $E_F$ is increased and this is probably due to the breaking of hexagonal symmetry.

In the case of NiAs-type FeSe, these minority spin states are nearly degenerate, but the lattice distortion removes this degeneracy and the e$_g$-states move to higher energy in MnP-type FeSe, the electronic energy is lowered and $E_F$ falls in the valley. One can see that the lattice distortion significantly decreases the DOS at $E_F$, and the MnP-type FeSe has a lower DOS at $E_F$ than NiAs-type FeSe. In the case
of CsCl-type FeSe, the majority Fe $e_g$-states are completely occupied and the $t_{2g}$-states are partially occupied. Metallic conduction is mainly taken by the $t_{2g}$ spins in the majority as well as in the minority spin states. The total DOS shows mixing of the Fe d- and Se p-states. The total DOS of CuAu-type FeSe also shows metallic character; hybridization between the Fe d and Se p electrons can be seen. Note that both the $t_{2g}$ and the $e_g$ spins are completely occupied in the majority states. The exchange splitting between the $t_{2g}$ and $e_g$ spins in the majority state is weaker than in the minority spin states. We see that our calculated systems are metallic in the low and high pressure regions and the electronic structures agree with the previous experimental and theoretical data which suggests that the effect of onsite Coulomb interaction, i.e., LDA+$U$ type interaction, in FeSe will not have significant effects.

To shed more light on the structural phase transition of $\alpha$-FeSe and to see how the chemical bonding changes, the charge densities were also calculated and are plotted in figure 6 in a plane that contains both the Fe and Se atoms. The $\alpha$-FeSe phase forms an enhanced density on the side of the Fe atom. It is clear that the $\alpha$-FeSe bonds are more covalent, a bonding that causes the apparent deviation of the charge density contours from a spherical shape. Inside the Fe–Se block, the metal-like Fe–Fe (Se–Se) bonding occurs due to delocalized Fe 3d- (Se p-) states. Interestingly, similar bonding was also found in the FeAs superconductors [35]. Note that such a bonding is either absent or weak in the other crystal structures of FeSe. The structural transition to NiAs-type FeSe also changes the bonding character between the Fe and Se atoms. The charge density of NiAs-type FeSe, see figure 6(b), clearly shows that the bonding between the Fe and Se atoms is less covalent and the charges are more localized at the Fe and Se atoms and are nearly spherical. The bonding in MnP-type FeSe is similar to that in NiAs-type FeSe. In CsCl-type FeSe and CuAu-type FeSe the bonding becomes more ionic and the charge density becomes nearly spherical. It is obvious that the ionic interaction between the Fe–Se bonds becomes stronger and the covalent interaction becomes weaker when a structural phase transition occurs from $\alpha$-FeSe to the other phases of FeSe. We must note that the role of defects (Se or Fe vacancies) in FeSe cannot be ignored and such defects, which are usually in high energy states, may change the magnetic structure of FeSe [30]. The effect of Se/Fe vacancies on the structural phase transition of FeSe is beyond the scope of this work.

There might be a relation between superconductivity and covalency because $\alpha$-FeSe is more covalent than the other phases of FeSe, which have not yet shown superconductivity. The ground state structure of FeSe is NM $\alpha$-FeSe and
it does not show any magnetic or structural instability at zero pressure. The experimentally observed decrease in the \( T_c \) of \( \alpha \)-FeSe at high pressure \([6]\) might be due to a structural/magnetic instability because our calculations show that there is a structural and magnetic instability under high pressure and a structural phase transition takes place to non-superconducting FeSe, e.g., NiAs-type FeSe. Although there is no consensus on the mechanism of the observed superconductivity of \( \alpha \)-FeSe, the Fermi surface topology plays a crucial role \([36]\) in forming the mediating quasi-particles for Cooper pairs as in cuprates \([37]\). Once \( \alpha \)-FeSe transforms into the other structures, this Fermi surface topology and the corresponding van Hove singularity near the Fermi surface will not be maintained anymore. Therefore, the decrease in \( T_c \) at high pressure may be due to a structural/magnetic instability. This suggests that we may increase the \( T_c \) of FeSe if such a structural phase transition at high pressure is avoided. It may be suggested that the structural phase transition in \( \alpha \)-FeSe can be controlled by doping \([38, 39]\). Further work is necessary to control this phase transition or increase the transition pressure of \( \alpha \)-FeSe.

4. Summary

Using \textit{ab initio} calculations, we have shown the phase transition of superconducting \( \alpha \)-FeSe. The predicted structural phase transition and transition pressure were shown to be in excellent agreement with existing experimental observations. Our calculations also showed that there is a structural phase transition from NiAs-type to MnP-type and CsCl-type FeSe. The phase transition from MnP-type to CsCl-type FeSe requires larger pressure than that to NiAs-type FeSe. The electronic structure and charge density were similar to those

Figure 5. (Continued.)

Figure 6. Charge density contours of (a) \( \alpha \)-FeSe, (b) NiAs-, (c) MnP-, (d) CsCl-, and (e) CuAu-type FeSe in the planes containing Fe and Se atoms. The lowest contour starts from \( 2 \times 10^{-4} \) electrons per au\(^{-3} \) and the subsequent lines differ by a factor of \( \sqrt{2} \). The color code of the charge density contours is ordered as blue, green, yellow, and red, in ascending order. The dotted lines show the bonds between Fe and Se atoms.
of FeAs based superconductors. The calculations revealed that the covalent bond between Fe and Se becomes weaker and the ionic bond becomes stronger when $\alpha$-FeSe is transformed to other structures. The experimentally observed decrease in the $T_c$ of $\alpha$-FeSe at high pressure may be due to a structure/magnetic instability. A possible scenario for the enhancement of $T_c$ was also discussed.

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