Pressure induced Lifshitz transition in ThFeAsN

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Outline of talk

- Introduction
- Crystal structure of ThFeAsN
- Computational details
- Results
  - Structural parameters vs pressure
  - Electronic structure vs pressure
  - Evolution of FS with pressure
  - Effect of Spin-orbit coupling
- Conclusions

ThFeAsN

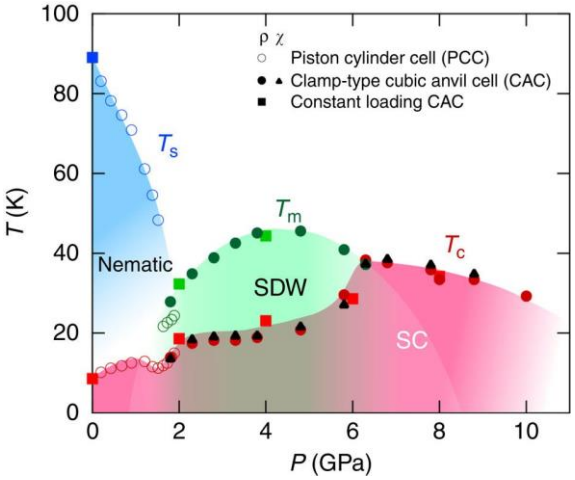
- ✓ ThFeAsN, a new member of 1111 Fe based SC (similar to LaFeAsO, the first Fe based SC) with a T_c of 30 K in the stochiometric compound in ambient pressure.
- ✓ No long range magnetic order has been found in ThFeAsN but a strong magnetic fluctuations above 35 K is observed.
- ✓ No structural transition.
- ✓ However a weak structural disorder at around 160 K is observed.
- ✓ Absence of long range magnetic order indicates that superconductivity may have some non magnetic origin.

Pressure and Superconductivity

- Pressure is an important control parameter that can effectively shrink the lattice, thus change the corresponding electronic states and transport properties.
- Almost all of the superconducting metallic elements (BCS el-ph coupled SCs) show a decrease of Tc with pressure.

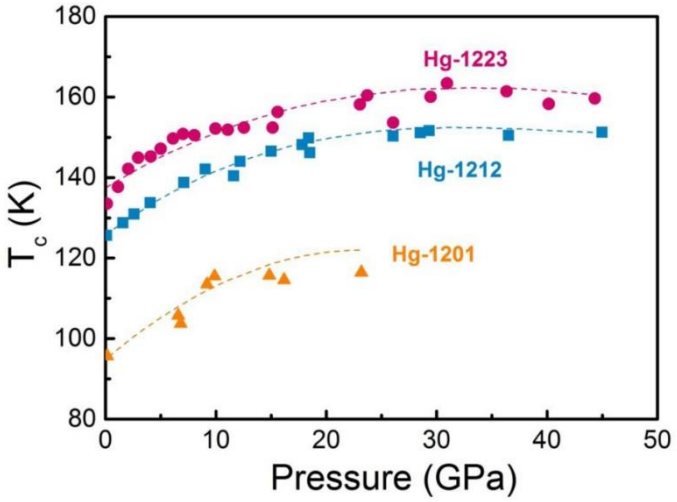
High temperature SCs Applying pressure to increase the T_c

FeSe



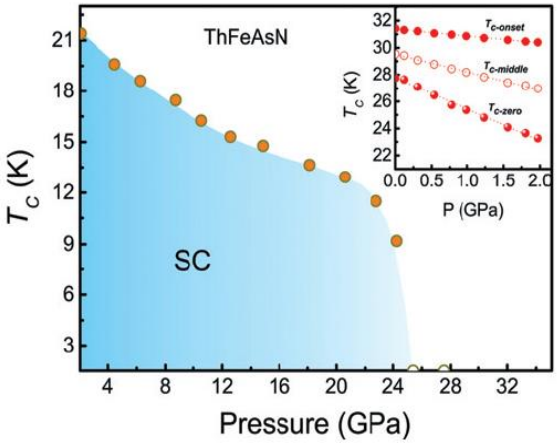
Nat. Commun. 7, 12146 (2016)

Cuprate superconductors



Phys. Rev. 50 4260 (1994)

ThFeAsN

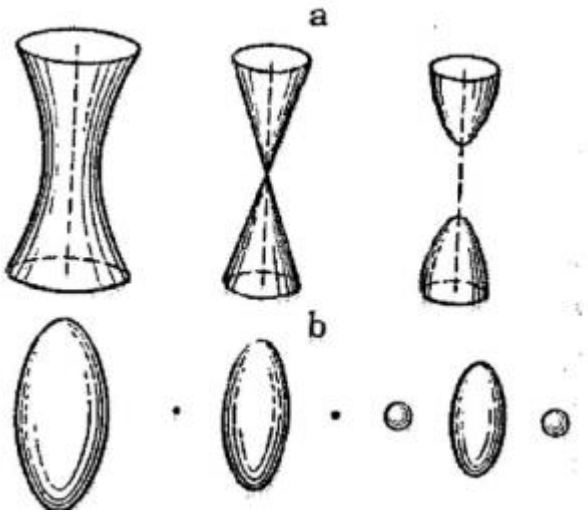


EPL **123** 67004 (2018)

What is Electronic topological transition or Lifshitz transition?

Lifshitz JETP (1960)

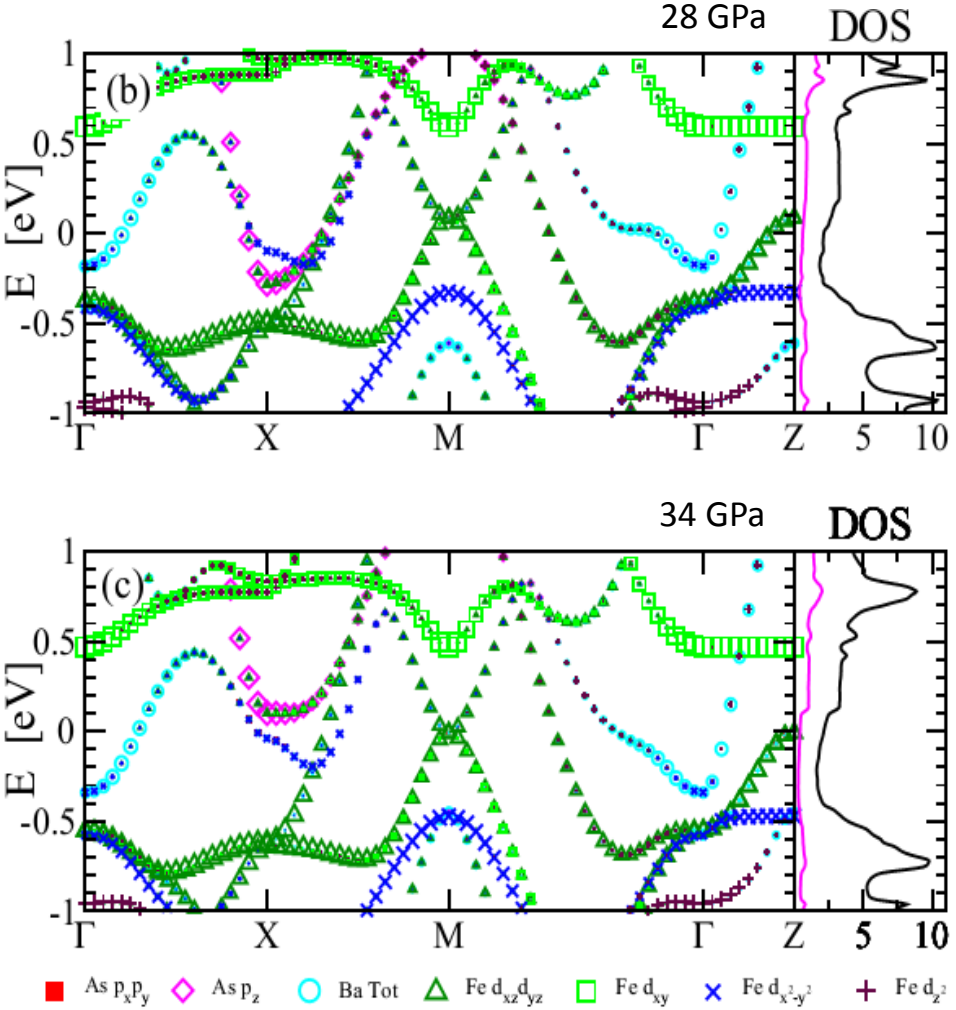
Electronic topological transition of the Fermi surface with no broken symmetries, known also as Lifshitz transition.



Lifshitz/ ETT in general can be doping driven, pressure driven, field driven.

Also, temperature driven.

Ref: Phys. Rev. Lett. 115, 166602 (2015).



$BaFe_2As_2$

Phys. Rev. B **90**, 144512 (2014)

What is the significance of LT?

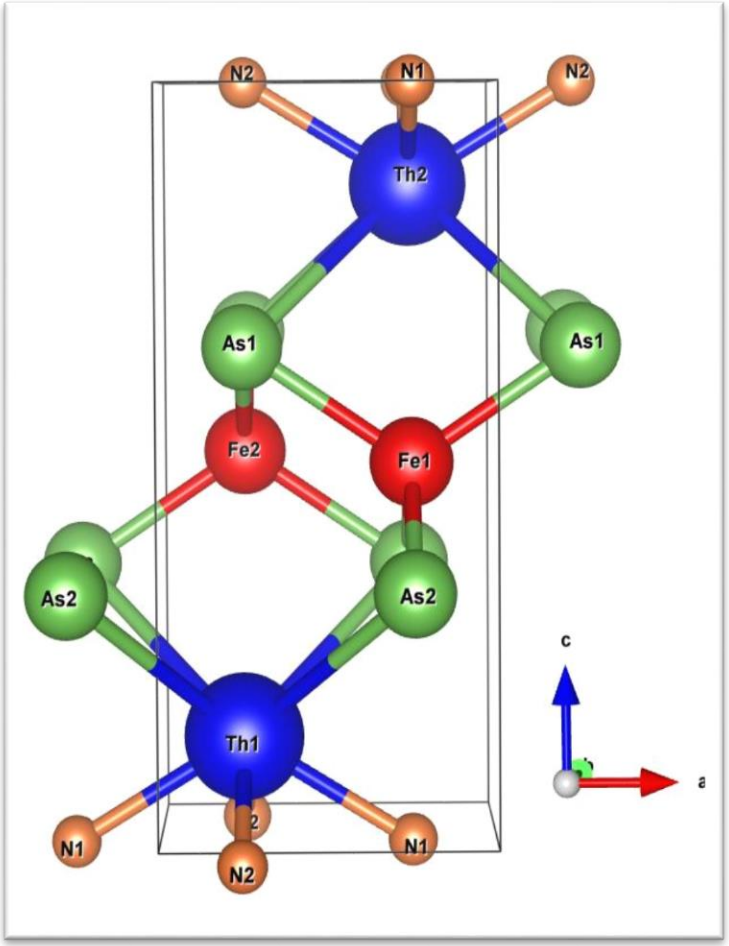
- LT can lead to reduced inter-band scattering (affecting mechanism of SC), nesting of FS (affecting magnetism), anomalies or singularities in the density of states near Fermi level (FL) and in general anomalies in the kinematics, dynamics and thermodynamics of electrons etc., which would affect various physical properties.

- Determining LT/ETT experimentally is challenging specially in systems that constitute multi-orbital-derived FS like Fe-based SCs or the current system.

- Close connection between LT and superconductivity is mentioned in literature [Journal of Physics and Chemistry of Solids 103 (2017) 170] but are high T_c superconductors topological or whether the high T_c is restricted by electronic topological transitions ?

- LT can be used to tune the T_c theoretically for Fe based SCs and can be a powerful tool to understand the mechanism.

Crystal Structures of ThFeAsN



- ✓ The compound crystallizes in a ZrCuSiAs-type structure
- ✓ 8 atom unit cell, space group P4/nmm, Tetragonal.
- ✓ The electrical resistivity and dc-magnetic susceptibility measurements indicate superconductivity at 30 K for the undoped ThFeAsN. [J. Am. Chem. Soc. 2016, 138, 2170−2173]
- ✓ No structural transitions

Computational Details

- Our first principles electronic structure calculations are carried out using plane wave pseudopotential method based on density functional theory (DFT) as implemented in VASP package.

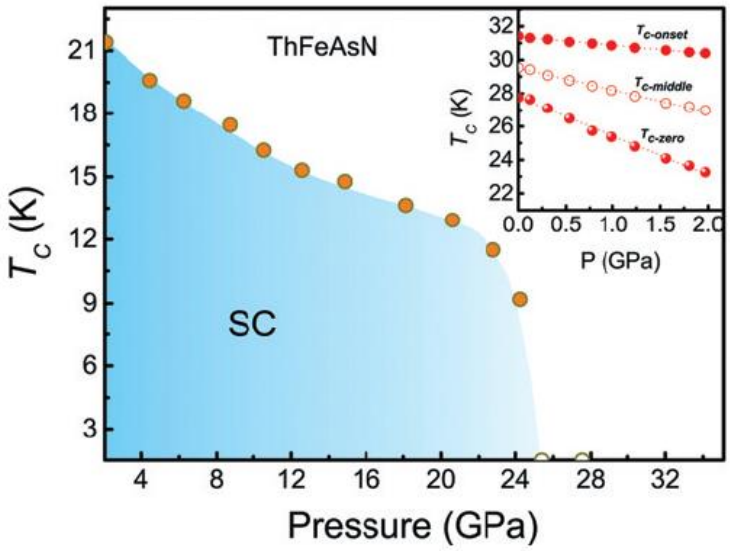
- Electronic exchange correlation is treated under the generalized gradient approximation (GGA) using Perdew–Burke–Ernzerhof (PBE) functional.

- We use plane-wave basis set with energy cut off 600 eV, self-consistent field (SCF) tolerance as 10^{-6} eV/atom and k-point grid 12x12x6 centered at gamma point.

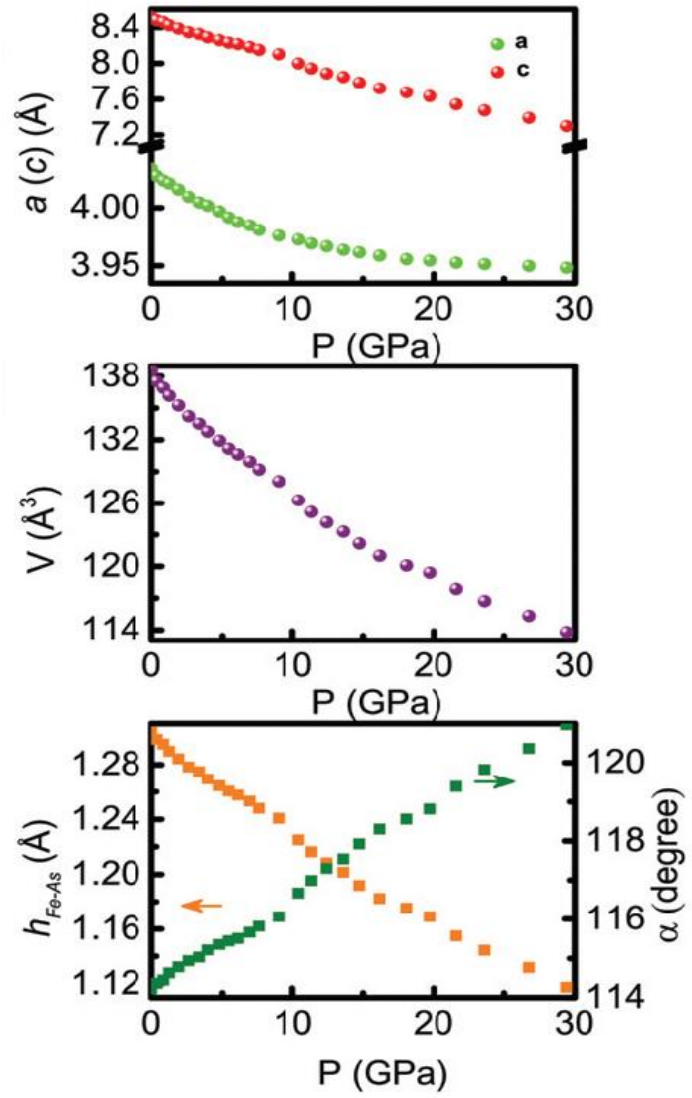
- For Fermi surface calculations, denser k-grid is used.

Effect of pressure in ThFeAsN (Expt.)

Phase Diagram



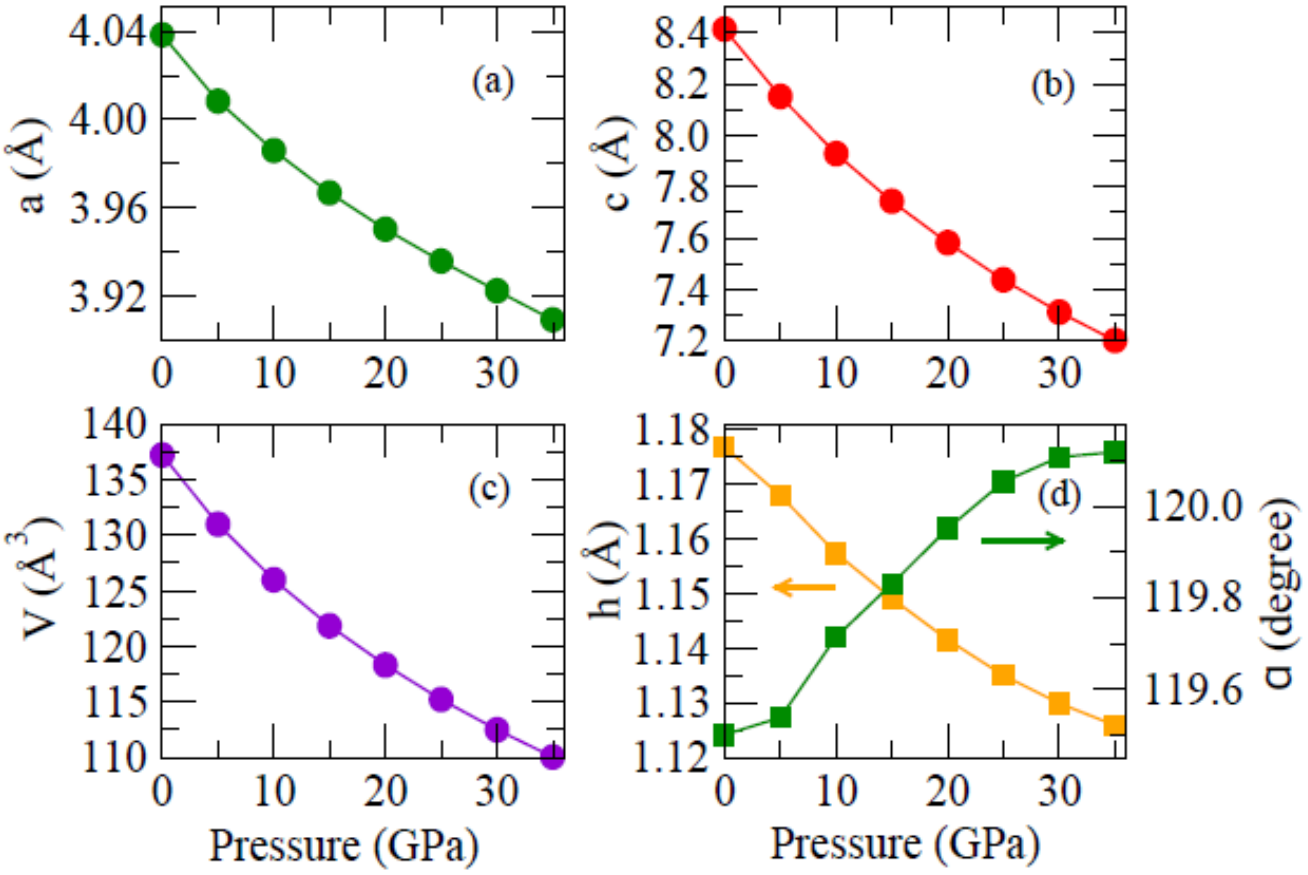
Structural Parameters



- ✓ No pressure-induced structural phase transition is observed in ThFeAsN up to 29.4GPa
- ✓ Tc is decreasing with increasing pressure!

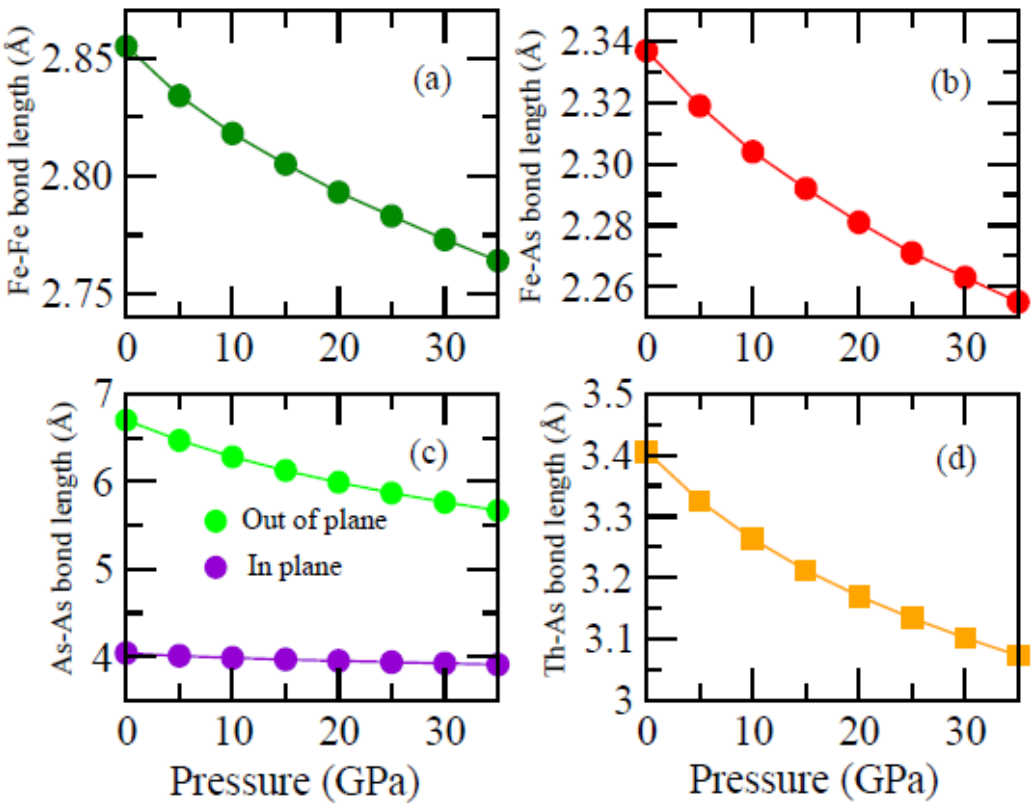
Wang *et al* 2018 *EPL* **123** 67004

Structural parameters vs Pressure (Theory)



Our calculated results are consistent with the experimental trends.

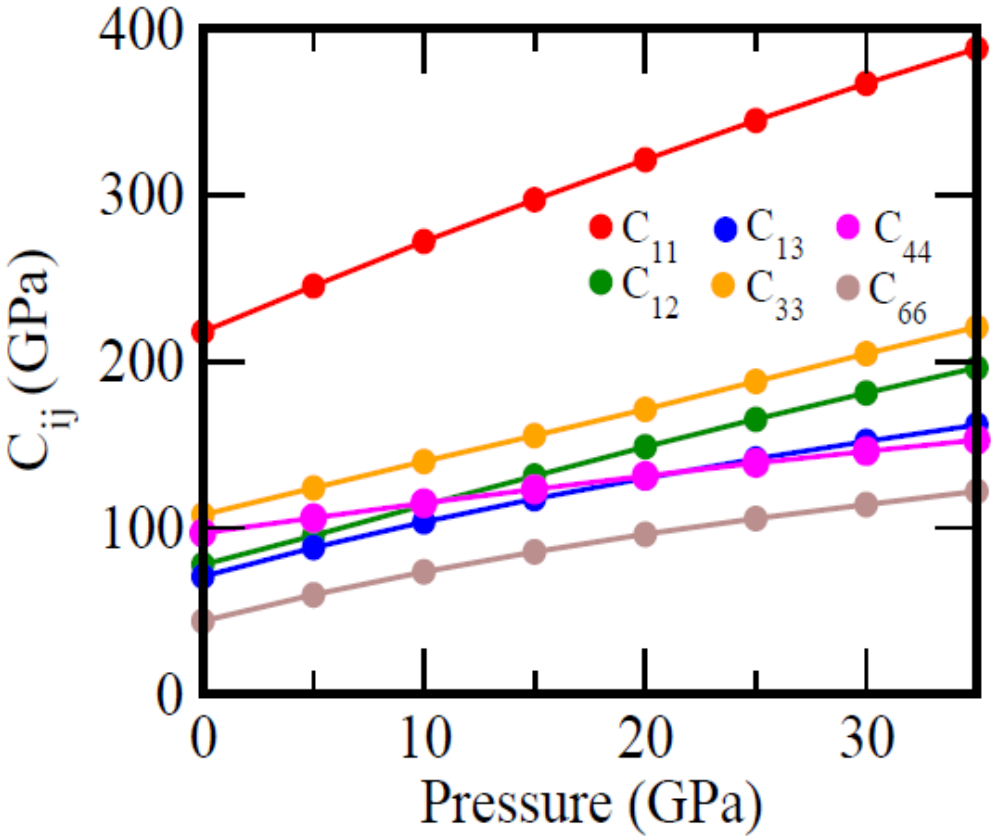
Structural parameters vs Pressure (Theory)



- Variation of out of plane As-As distance is more prominent than that of the in plane one.

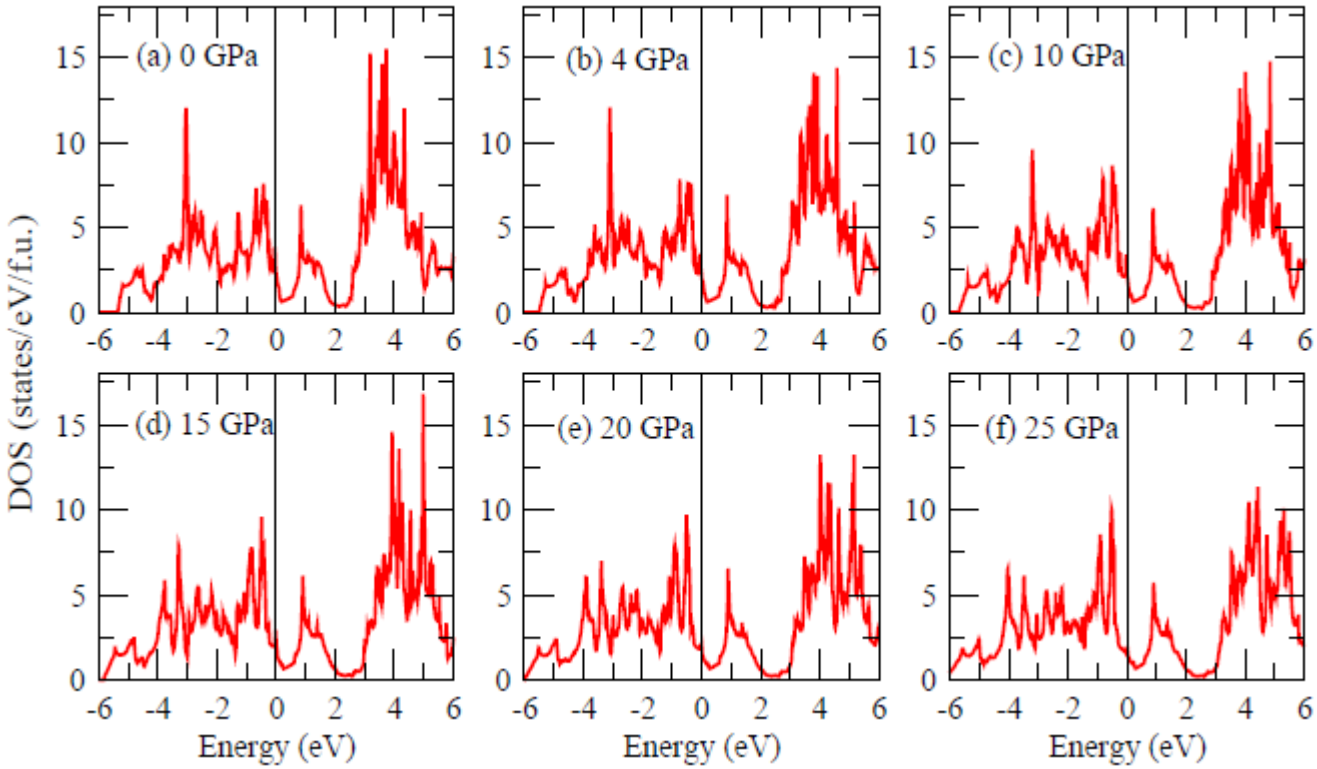
- This indicate that there is significant modifications along the c axis as compared to that in the ab plane.

Elastic constant vs Pressure (Theory)



No structural transition!

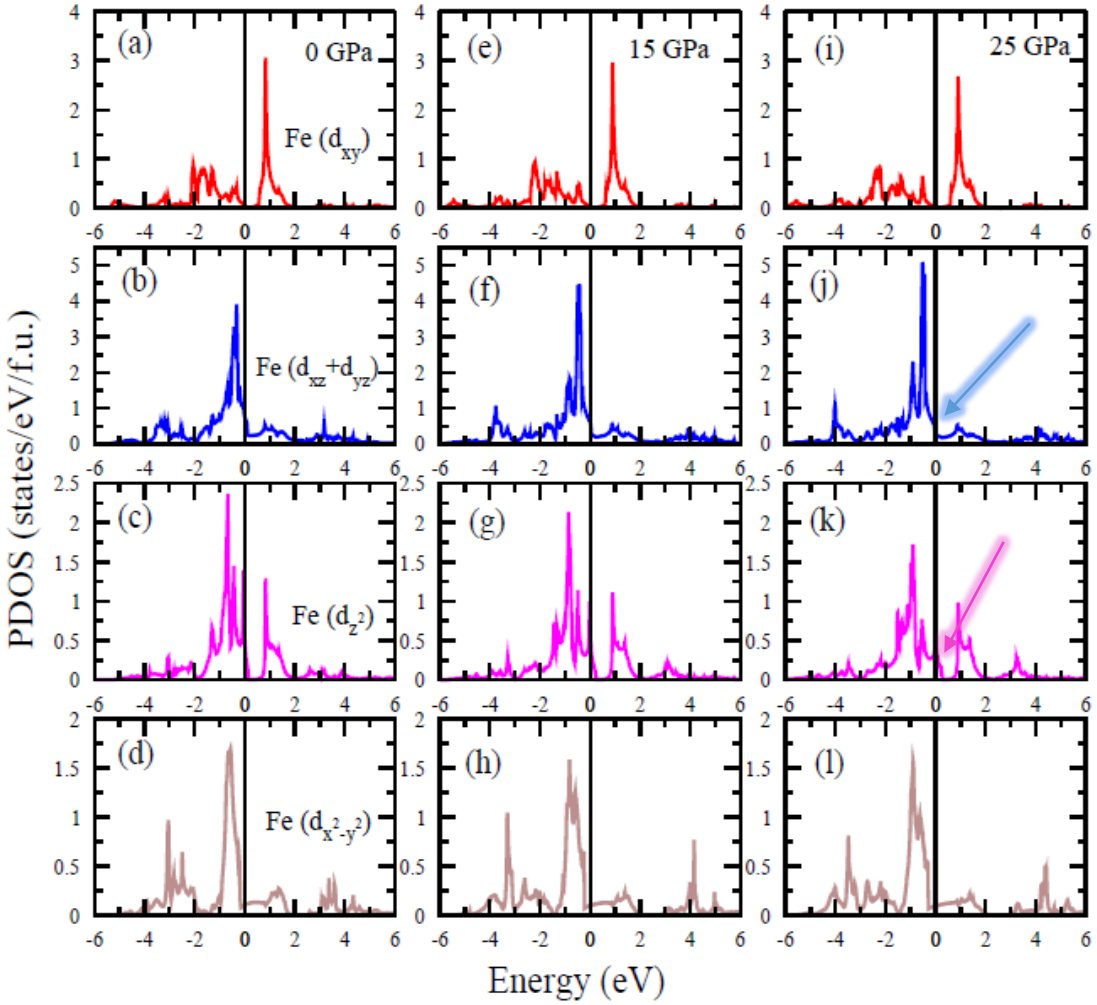
Density of states vs Pressure



- Fermi level shifts towards unoccupied states as we go towards higher pressure.

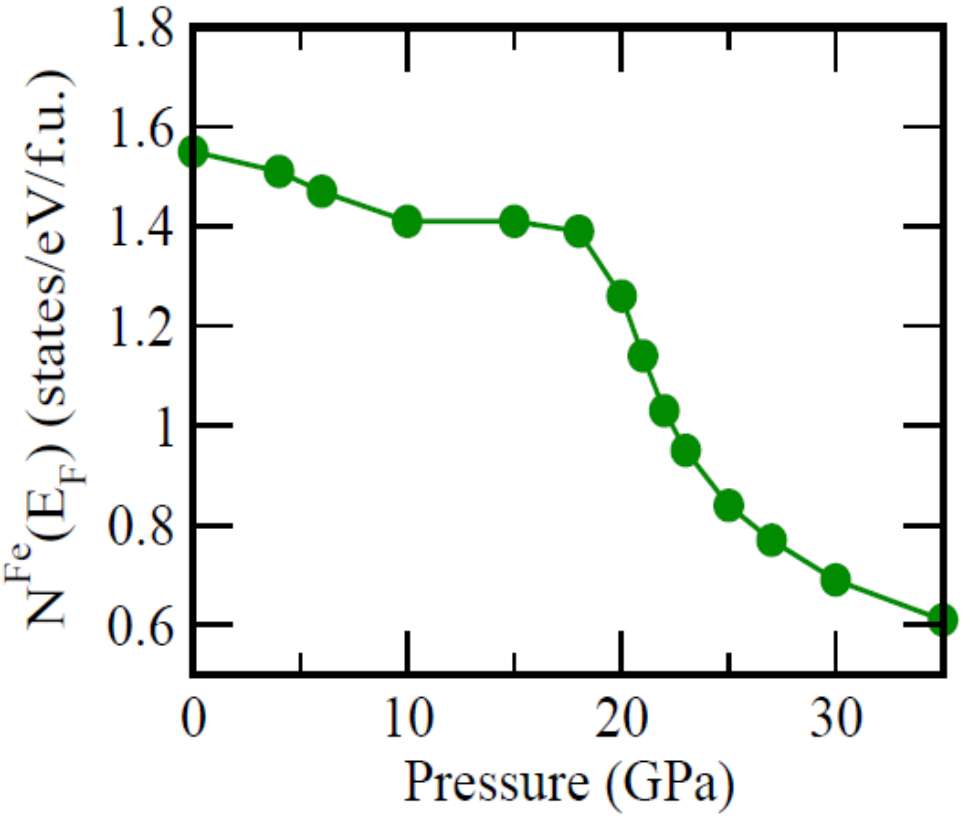
- This scenario is very similar to electron doping within rigid band model.

Fe-d orbital projected Density of states



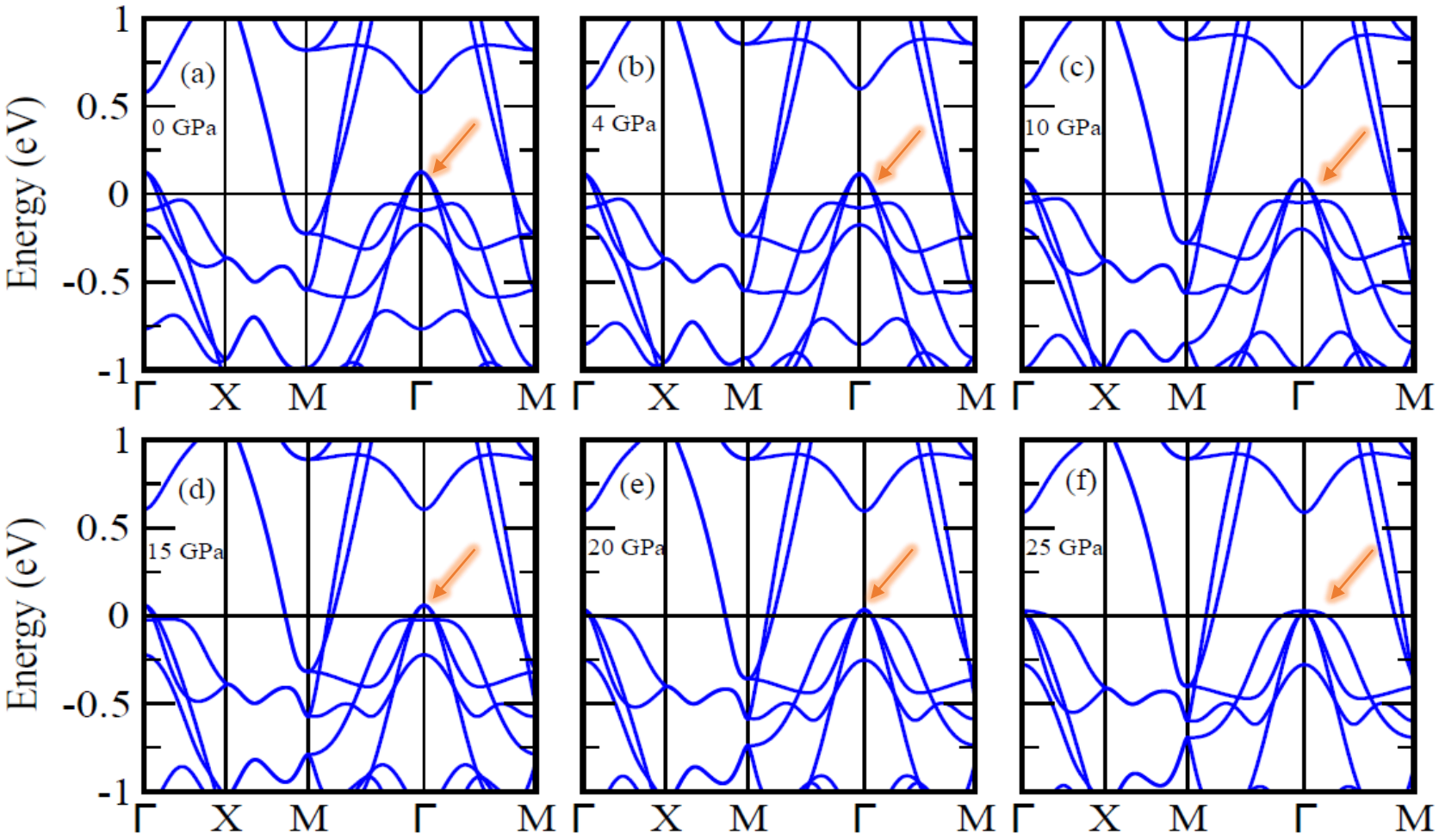
Fe-d orbital derived partial DOS are modified remarkably with pressure as the Fermi level shifts away from a van Hove singularity as we go towards higher pressure.

Density of states (Fe) at Fermi level



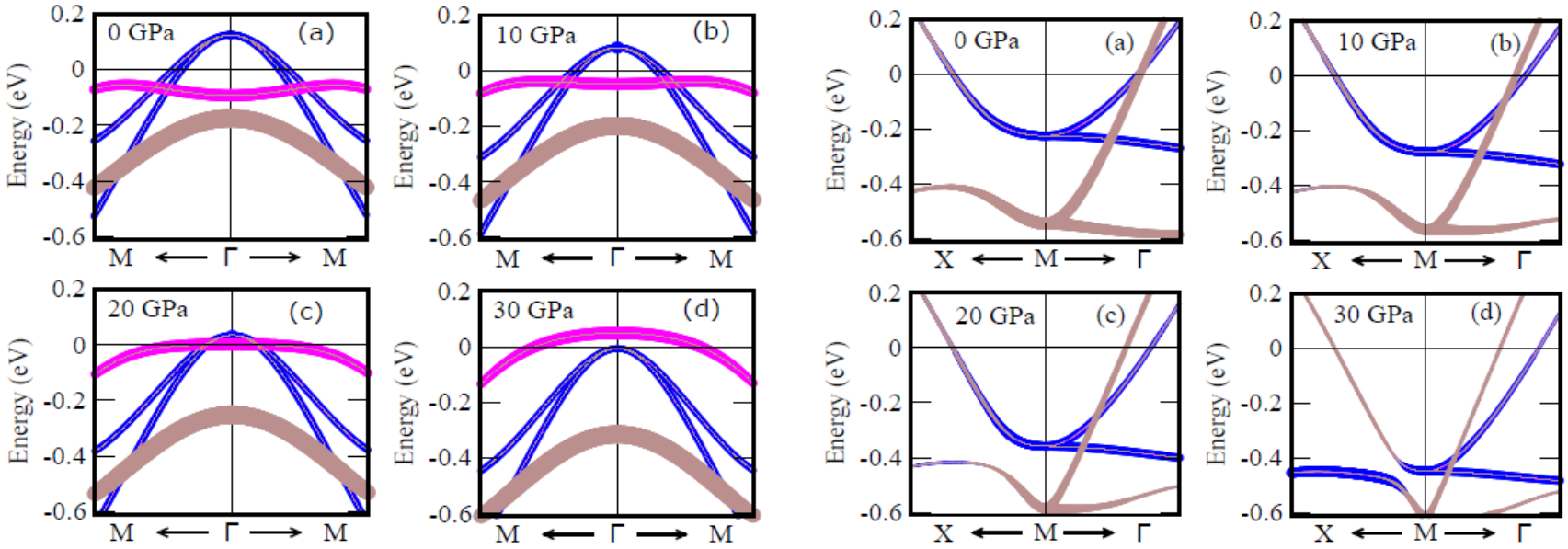
- ✓ $N_{E_F}(\mathrm{Fe})$ **is decreasing with increasing pressure.**
- ✓ **Decrease the possibility of electron pairing.**

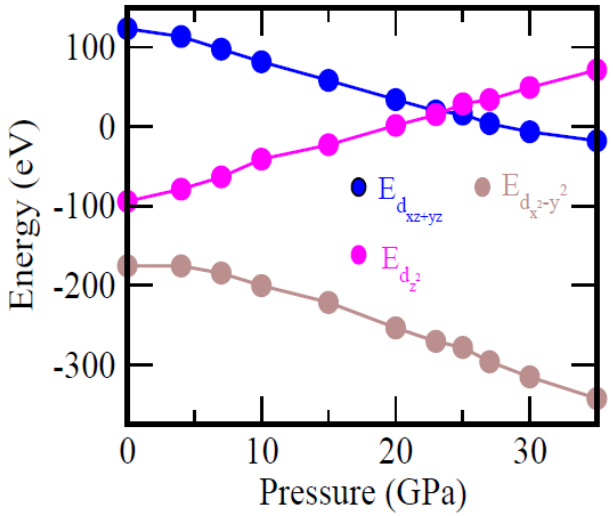
Band structures at various pressures



A number of noticeable modifications are observed in the band structures at various hydrostatic pressures.

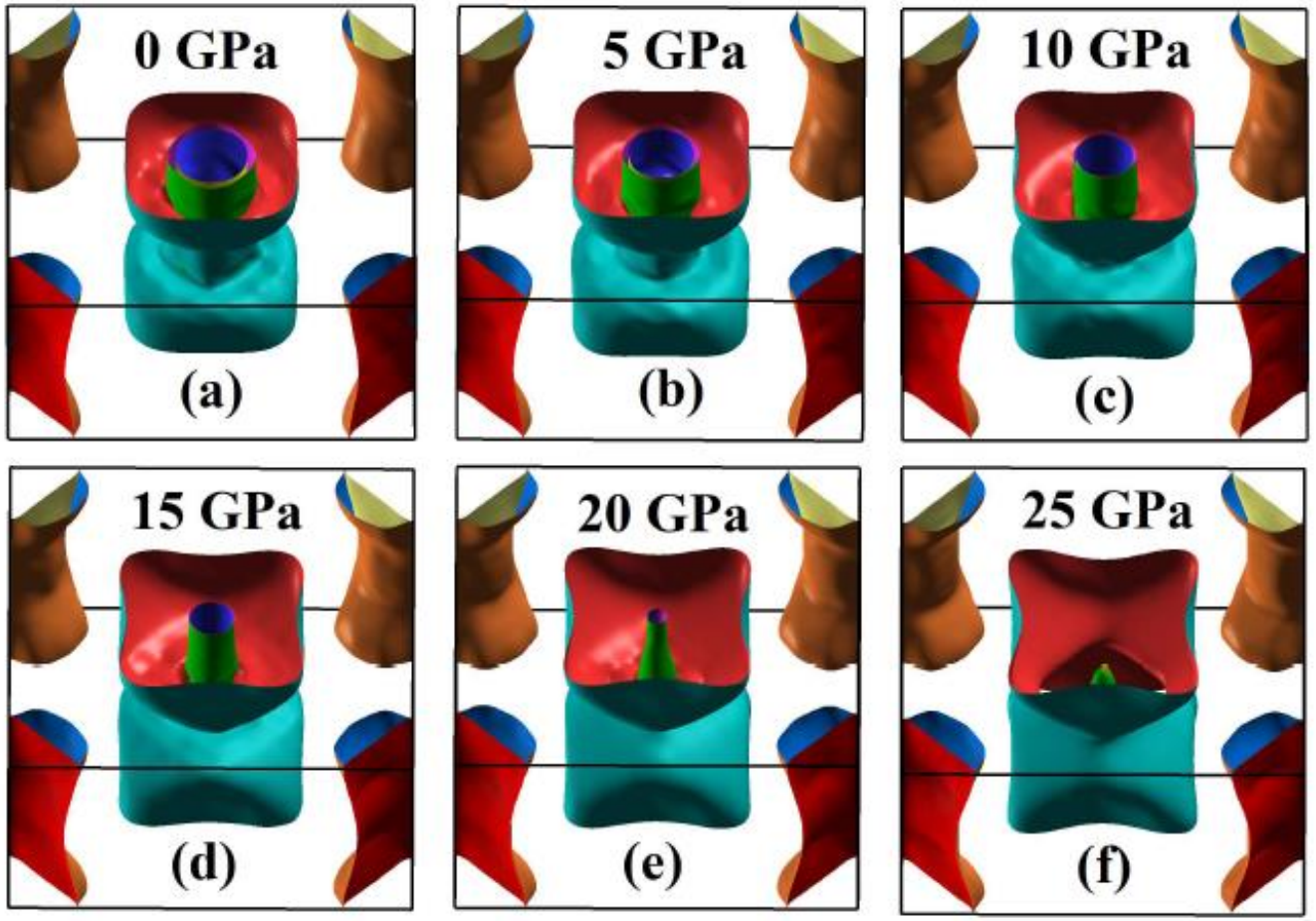
Lifshitz transition





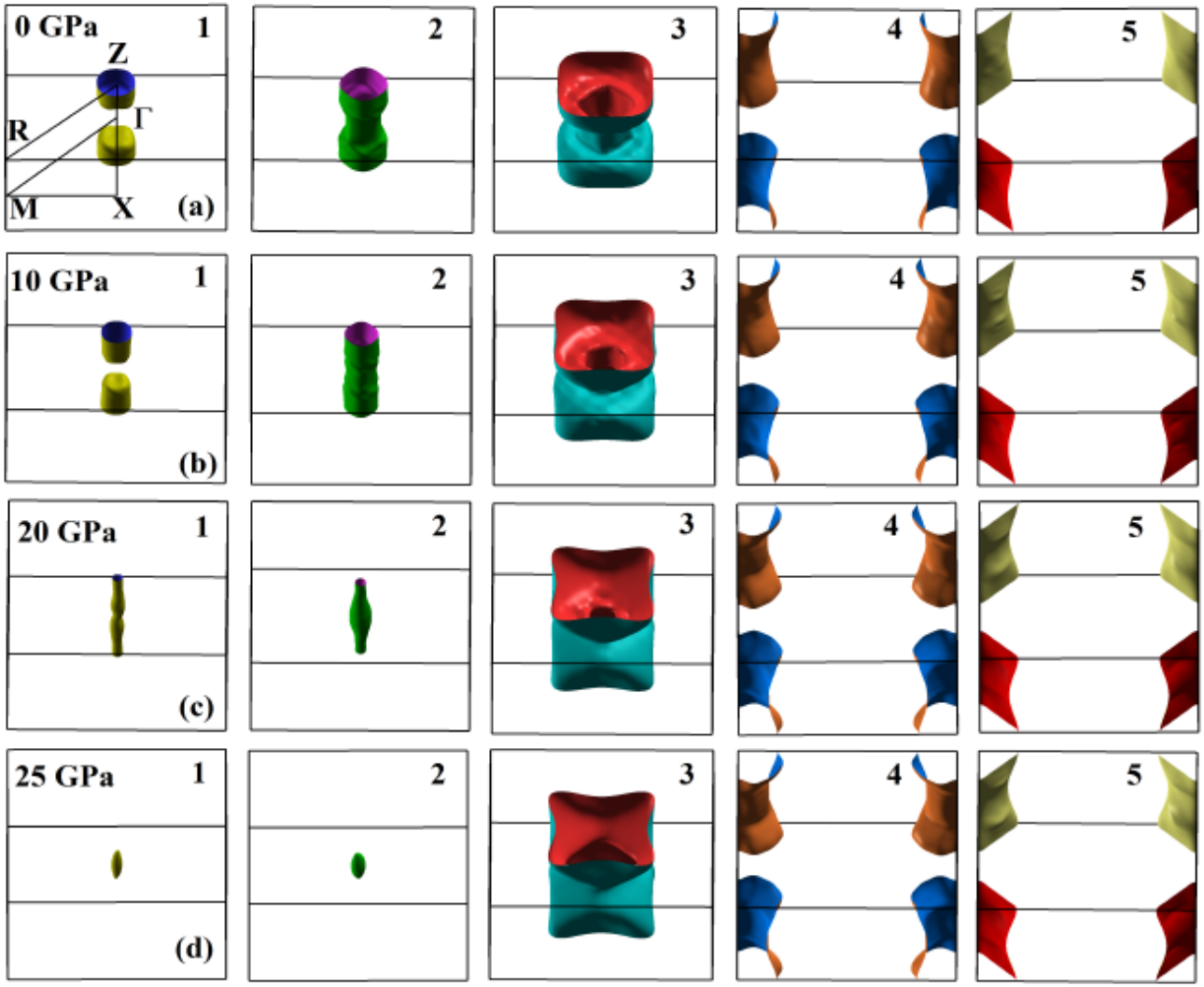
- Electronic bands around Γ point significantly modified as we gradually increase the pressure.
- Orbital selective Lifshitz transition.

Evolution of FS with pressure



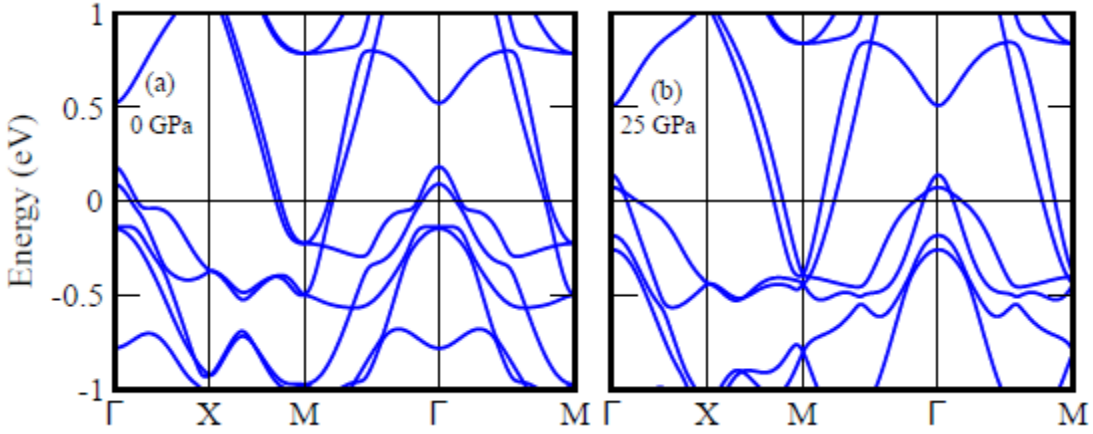
- Lifshitz transition in the hole like band at centre (Gamma point)
- There is no change in the electron like FSs with pressure

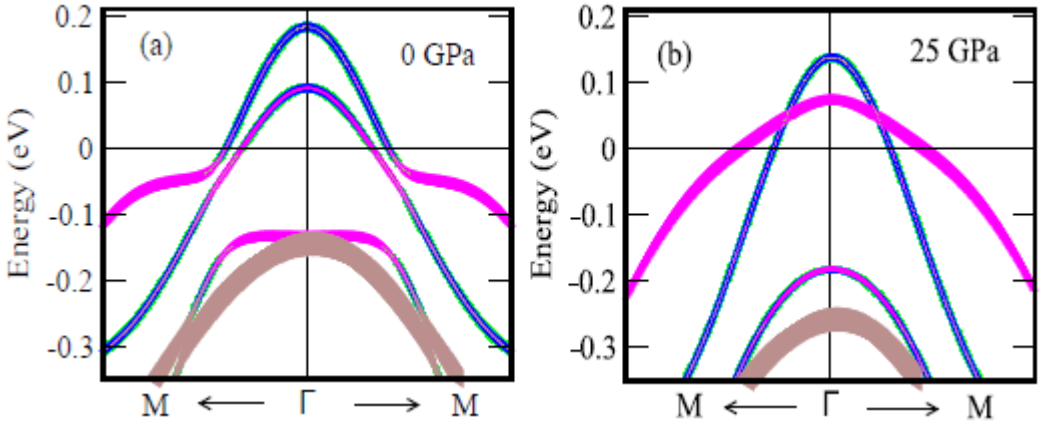
Evolution of all FSs separately with pressure



This evolution of FSs with hydrostatic pressure directly affect the nesting of FS, which is believed to play a key role in superconductivity of Fe-based SCs.

Effect of Spin-orbit coupling





Band dispersion around Γ point

LT also occurs in presence of SOC

Conclusions

- Structural parameters as well as elastic constants show no anomalous behaviour with hydrostatic pressure which is consistent with the experimental observation of absence of structural transition with pressure in ThFeAsN system.

- Density of states at the Fermi level, coming from Fe-d orbitals and superconducting T_c both varies similarly with pressure.

- We find a pressure induced orbital selective LT in ThFeAsN compound. This electronic topological transition or LT is quite different by nature from the Lifshitz transitions observed in the other families of Fe-based superconductor.

- Pressure dependent modification of FS topology which is nothing but the manifestation of LT observed in the electronic band structure at higher pressure, is mainly responsible for the reduction of superconducting T_c in ThFeAsN superconductor.

- In presence of SOC, LT still occurs at higher pressure. However, a change in the energy ordering of the orbitals is observed at higher pressure with the introduction of SOC.

Thank You