Helical Spin Order in $SrFeO_3$ and $BaFeO_3$

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Z. L. et al., PRB, 85, 134419 (2012)
Z. L. et al., PRB, 86, 094422 (2012)
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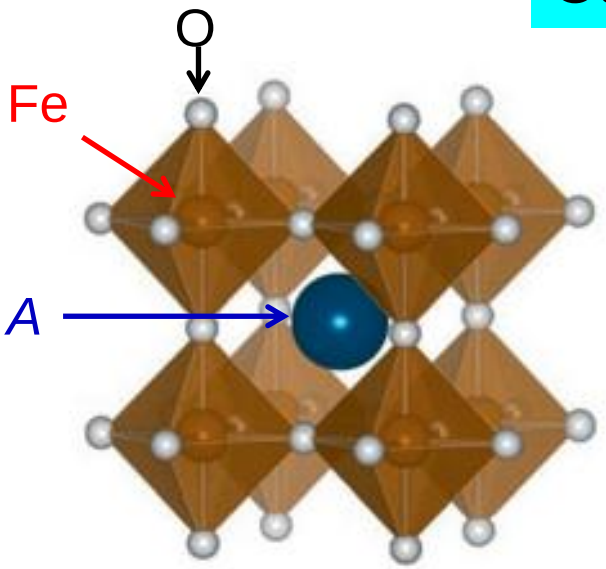
Outline

1. Introduction
2. Motivation and Purpose
3. Helical spin order in $BaFeO_3$ by first principles and model calculation
4. Phase transition driven by pressure
5. Open question: Helimagnet under magnetic field
5. Conclusion

Cubic provskite $AFeO_3$



A^{2+} A=Ca, Sr, Ba

O^{2-}

Fe^{4+} high valence $3d^4$

[A. E. Bocquet *et al*., PRB **45**, 1561 (1992)]

Coulomb interaction on Fe U_{eff}

$U_{eff}=E(3d^5)+E(3d^3)-2E(3d^4)$

~ 7eV

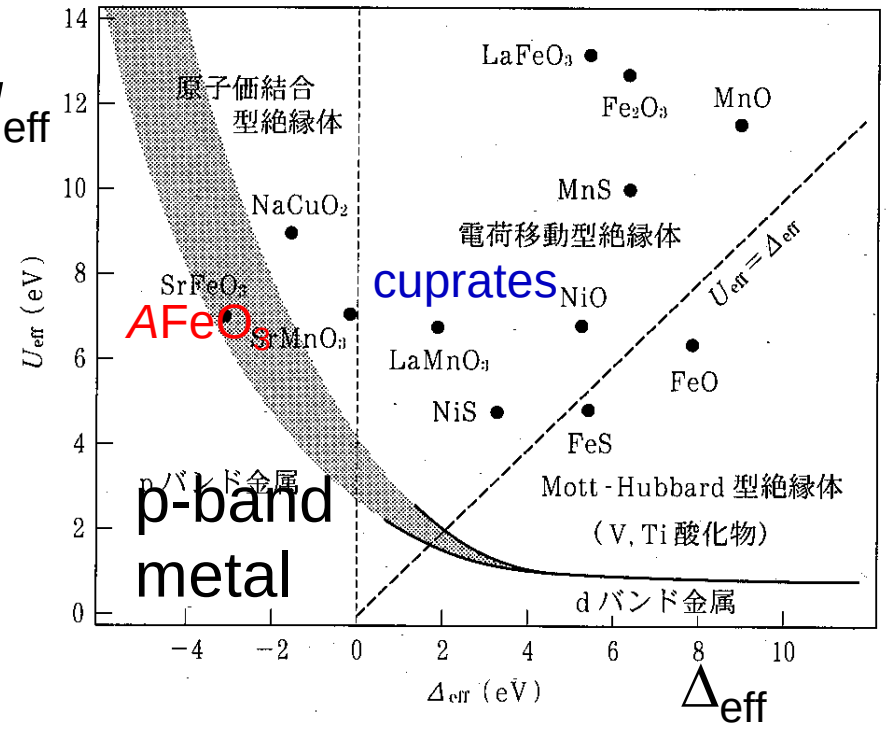
charge-transfer energy

$\Delta_{eff}=E(3d^5\underline{L})-E(3d^4)$

~ - 3eV

negative Δ material

Zaanen-Sawatzky-Allen diagram
[Can. J. Phys. 65, 1292 (1987)]



Introduction

Hallmark of $AFeO_3$ (A=Ca, Sr, Ba):Helical spin order and *p*-type metal, i.e. O2*p* electron makes main contribution to conductivity

In spherical coordinate, spin moment as :

$$S_i = S(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i)$$

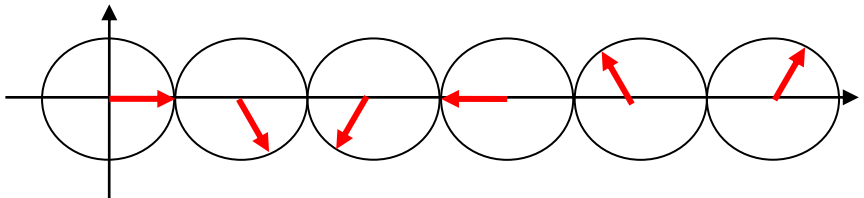
For helical spin order, the constraint is:

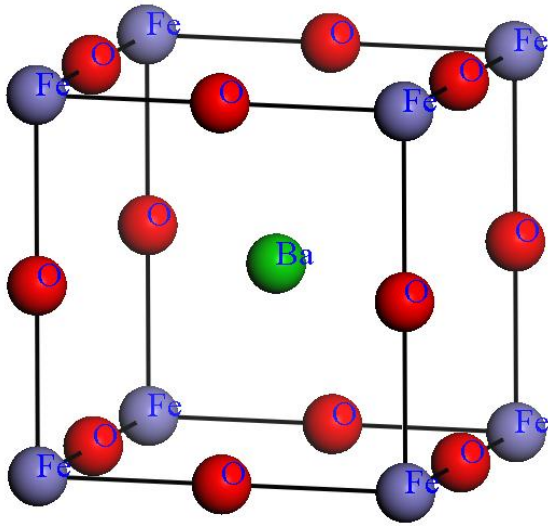
$$\theta_i = \vec{q} \cdot \vec{r}_i \qquad \phi_i = 0$$

Propagating vector $\vec{q}$ defined in reciprocal space

A-type helical spin $\vec{q} = \phi(1,0,0)$

G-type helical spin $\vec{q} = \phi(1,1,1)$





Motivation and Purpose

Experiment:

	T_N (K)	q (2π/a)
$CaFeO_3$	115	0.167(1,1,1)
$SrFeO_3$	134	0.112(1,1,1)
$BaFeO_3$	110	0.06(1,0,0) (*)

A-type

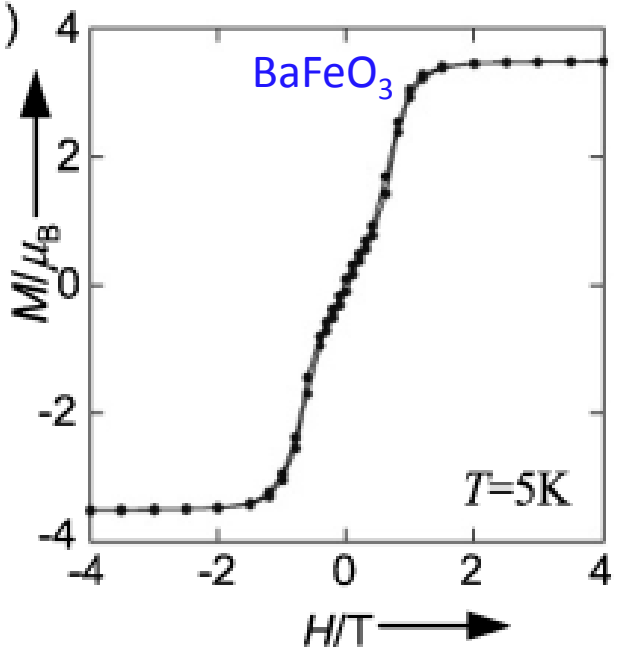
$$\mathbf{q} = \phi(1,1,1) \times 2\pi/a_S$$

N. Hayashi et al., Angew. Chem. Int. Ed. **50, 12547 (2011)**

Lattice parameter

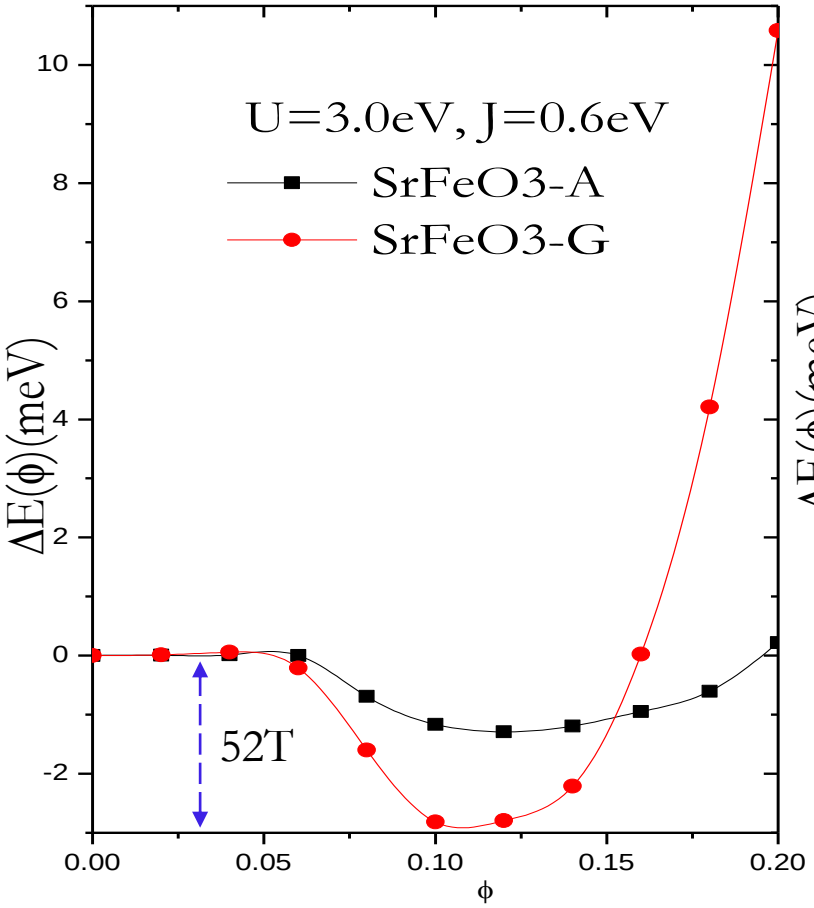
$SrFeO_3$: 3.85 Å

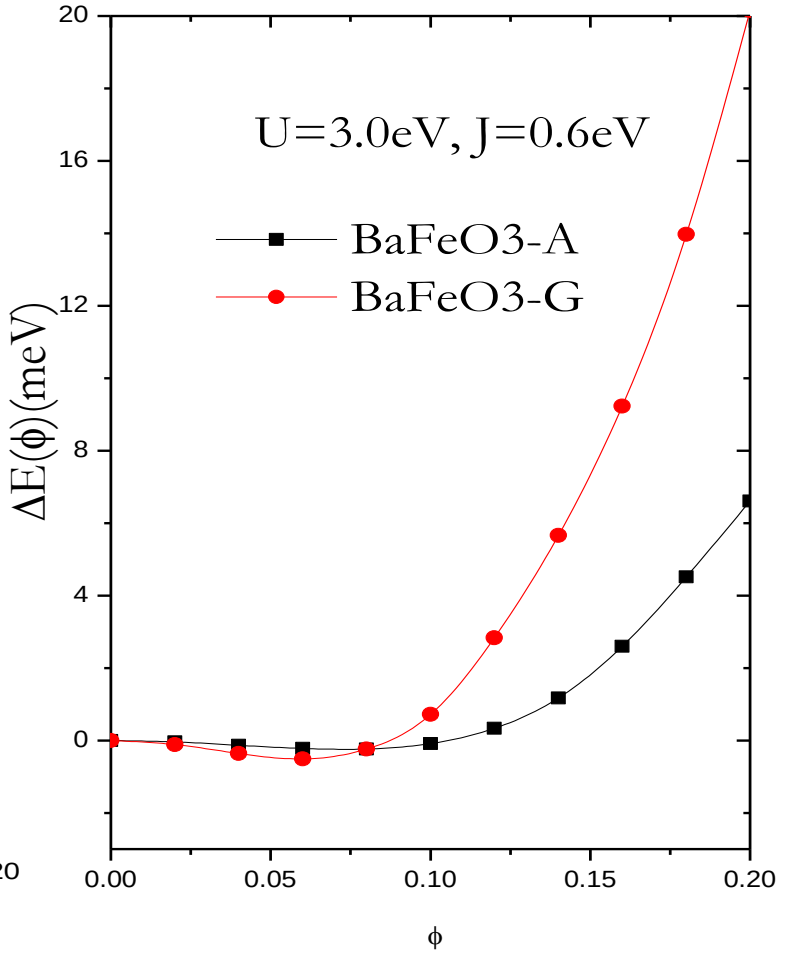
$BaFeO_3$:3.97 Å



DFT calculation

- Helical spin order predicted by local spin density approximation plus Hubbard U (LSDA+U) with generalized Bloch boundary condition





Physics behind the difference between $SrFeO_3$ and $BaFeO_3$?

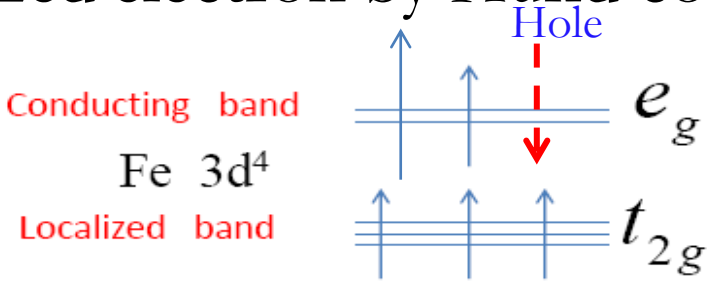
DFT calculation

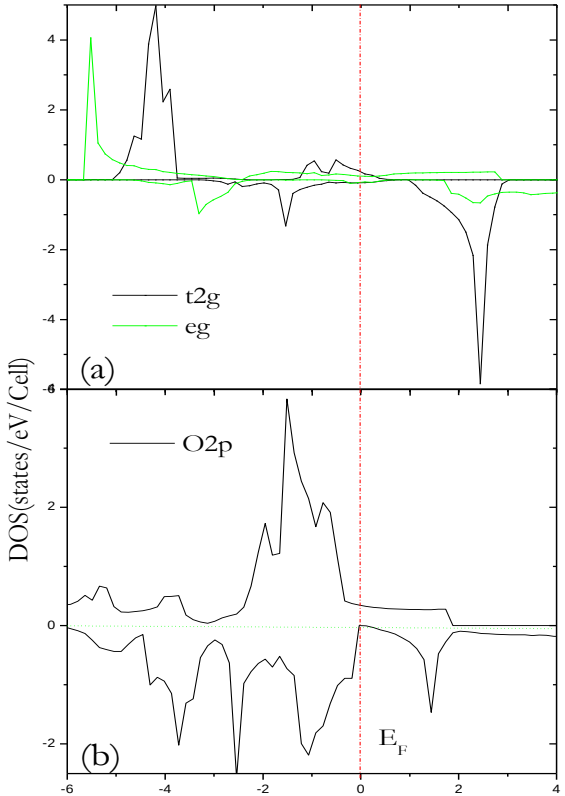
The density of state (DOS) of FM state in $BaFeO_3$ is calculate by LSDA+U, U=3.0eV and J=0.6eV

1.O2*p* makes the main contribution to density around the Fermi Level

2. Half-metallic

3. The system can be simplified as conducting electron coupled to localized electron by Hund coupling





Model calculation

It is reasonable to understand the calculated result from the double exchange model.

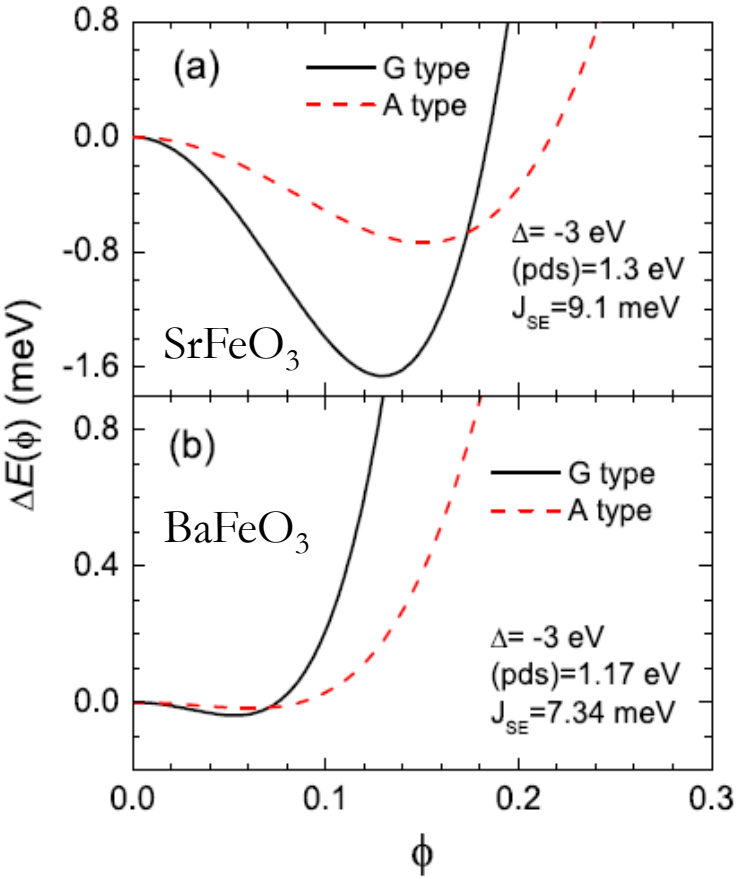
$$H = H_{dp} + H_{SE}$$

$$H_{dp} = \sum_{j\alpha b} t_{\alpha b}(d^{\dagger}_{j\alpha} u^{\dagger}_{j} P_{jb} + P^{\dagger}_{jb} u_j d_{j\alpha}) + t_{pp} \sum_{j,b\neq c} P^{\dagger}_{jb} P_{jc} + \Delta \sum_{jb} p^{\dagger}_{j+b/2} p_{j+b/2},$$

$$P_{jb} = p_{j+b/2} + p_{j-b/2}$$

$$H_{SE} = J_{SE} \sum_{<ij>} S_i \cdot S_j$$

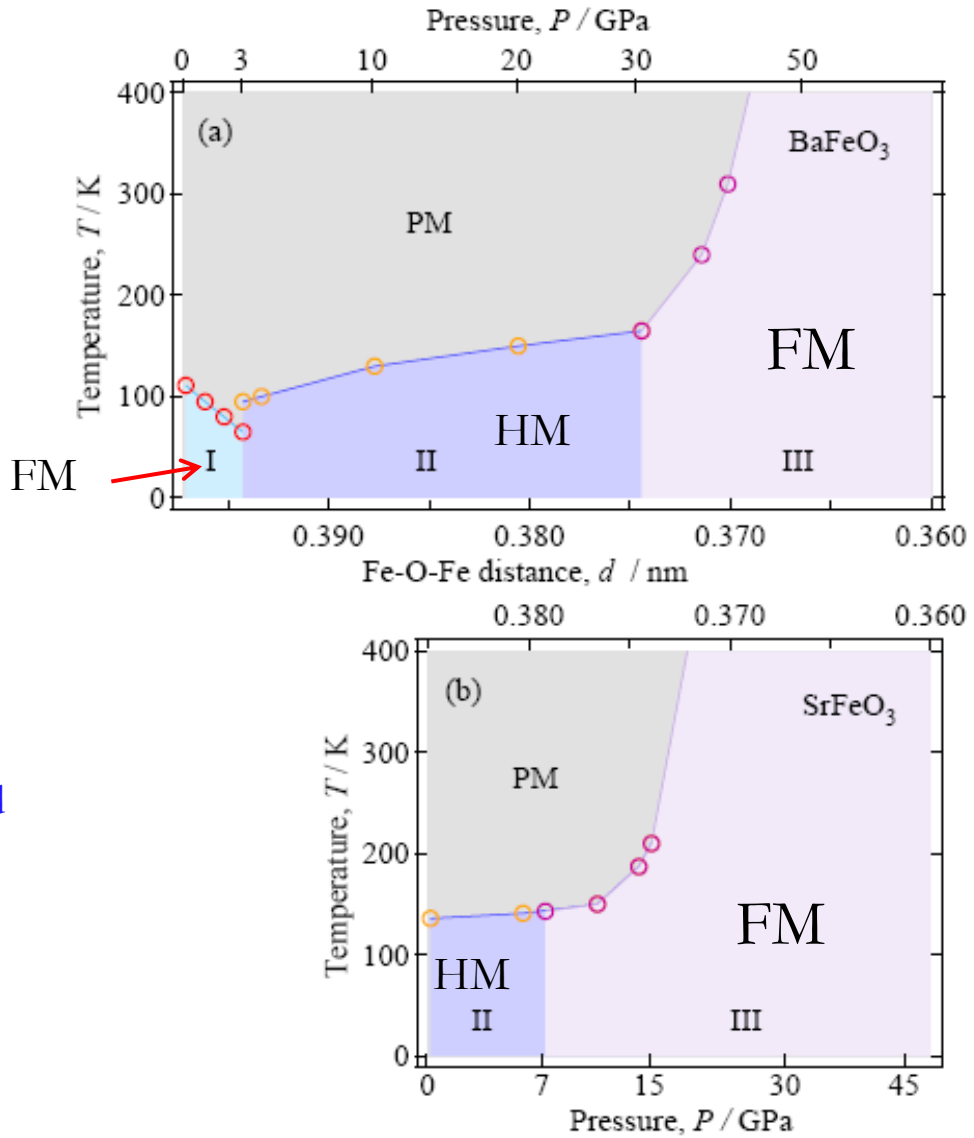
$$\mathbf{S}_j = S\left(\hat{z}\cos \mathbf{Q}\cdot\mathbf{x}_j + \hat{y}\sin \mathbf{Q}\cdot\mathbf{x}_j\right)$$



M. Mostovoy, Phys. Rev. Lett. **94, 137205 (2005)**

Phase transition driven by pressure

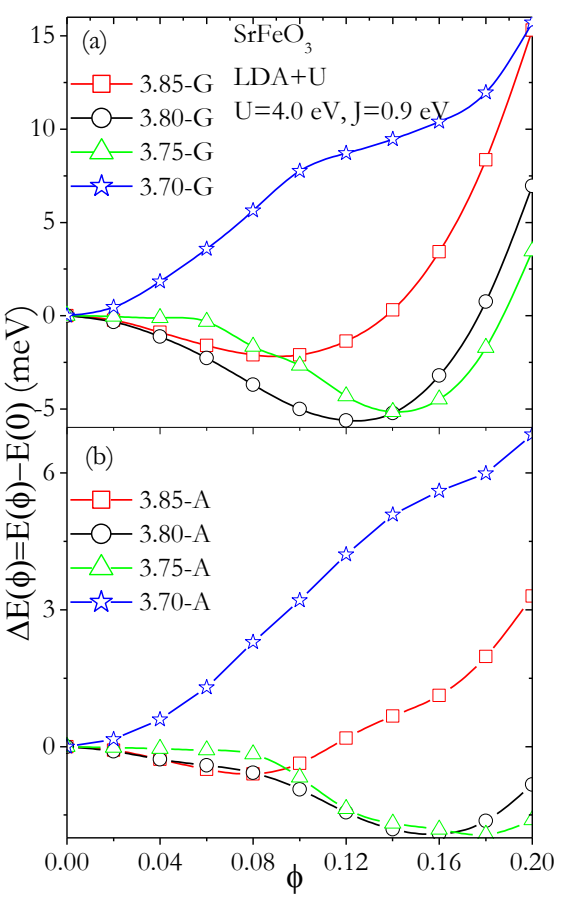
- Lattice effect

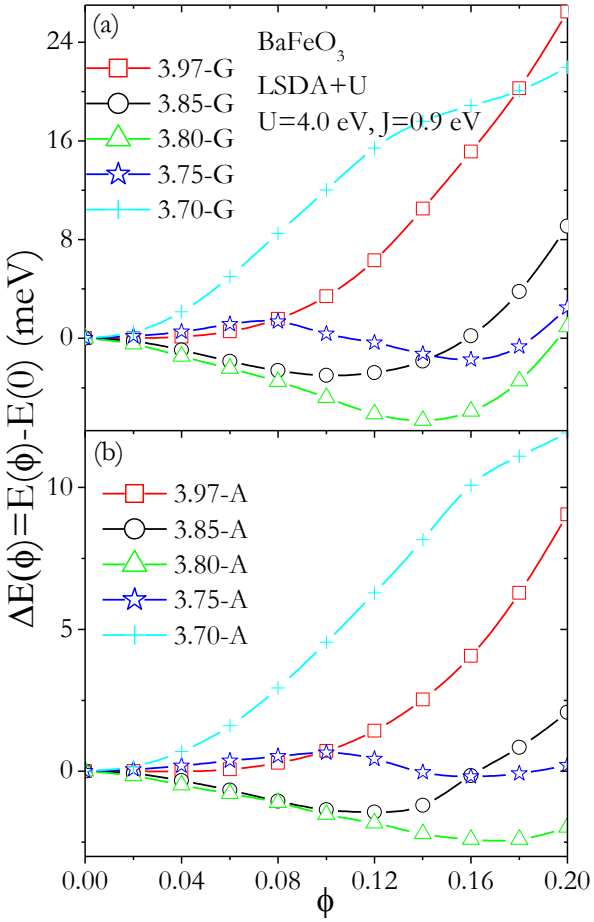


T. Kawakami et al., unpublished

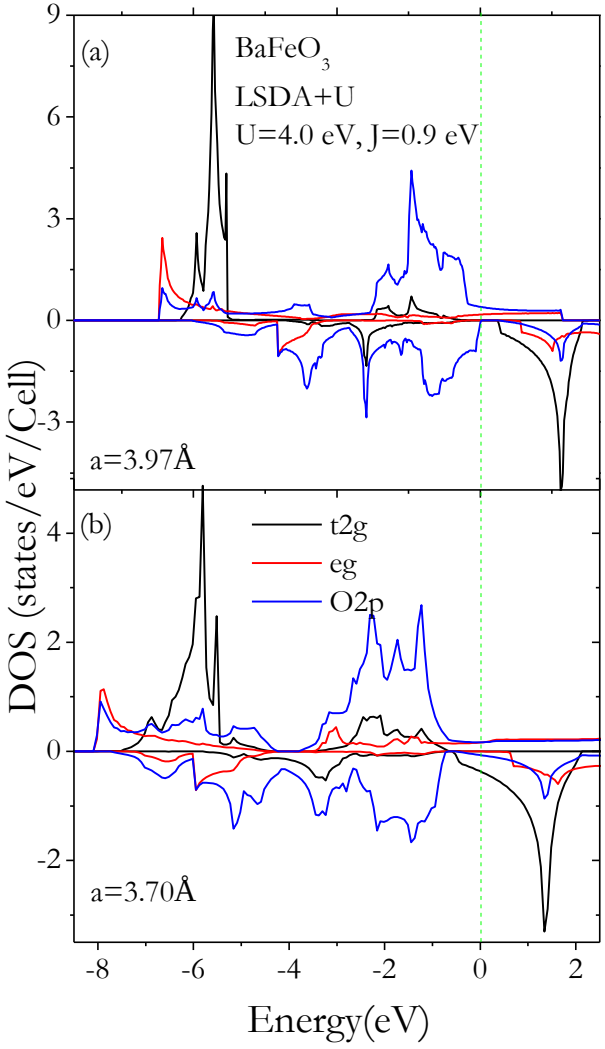
Phase transition driven by pressure

- Lattice effect by calculation





Phase transition driven by pressure

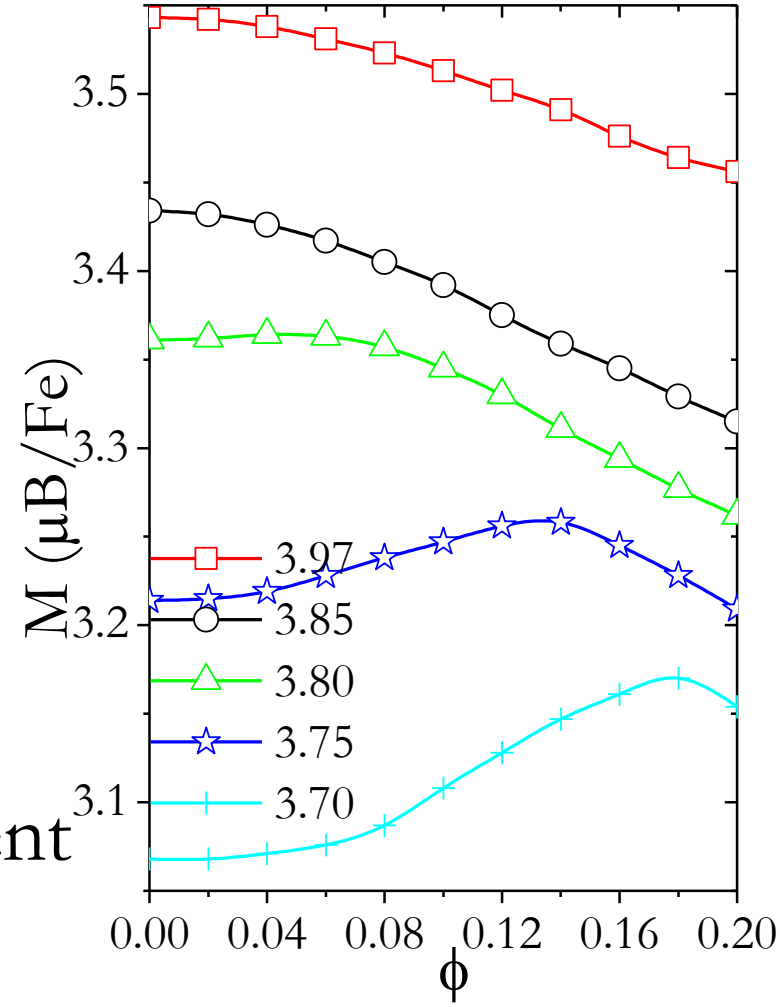


DOS

$$E_D \propto \frac{(pd\sigma)^2}{\Delta}$$

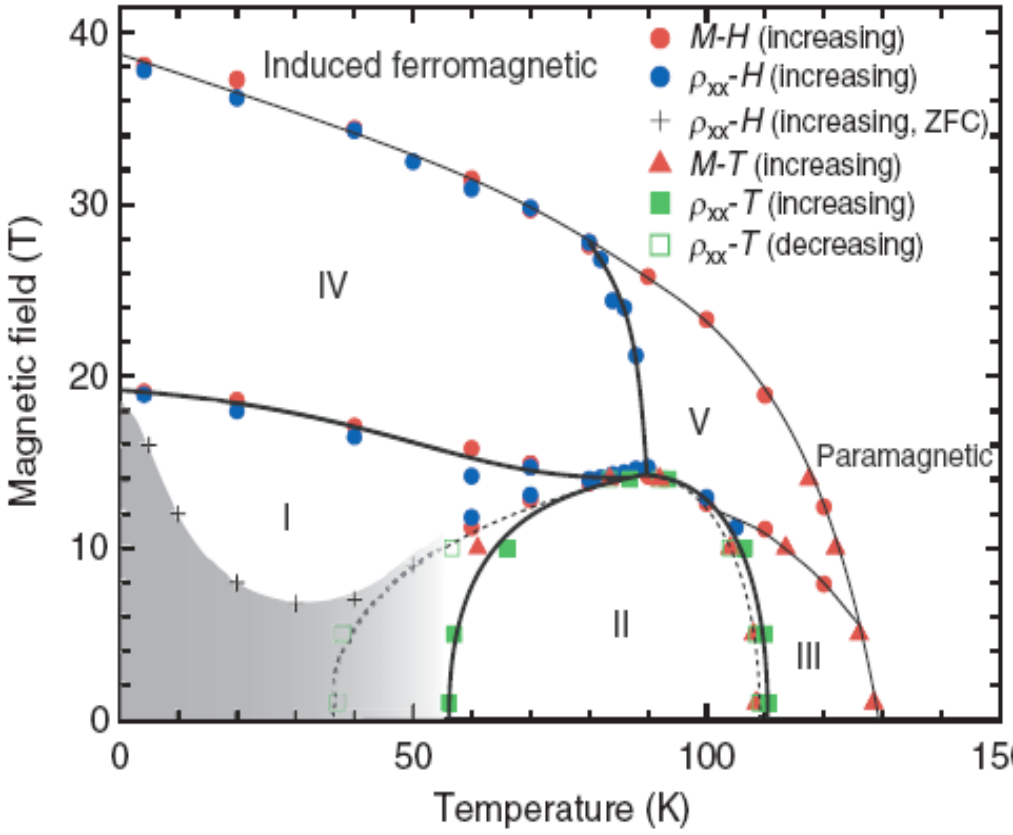
$$E_S \propto \frac{(pd\sigma)^4}{\Delta^2 U}$$

local moment

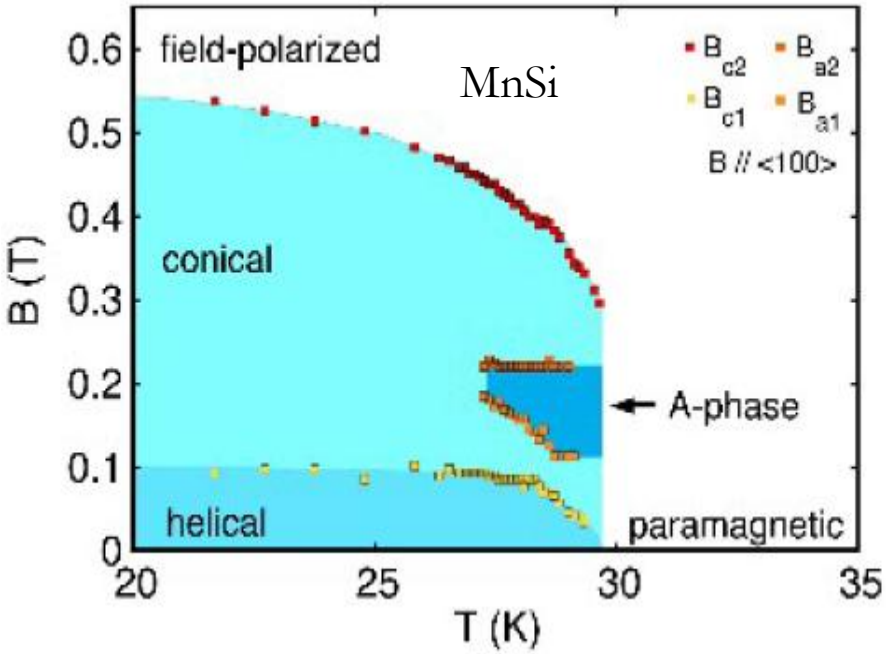


Open question

magnetic phase diagram and electronic transport in helimagnet $SrFeO_3$ under external field



S. Ishiwata *et al.*, Phys. Rev. B 84, 054427 (2011)



S. Mühlbauer *et al.*, Science, 323,915(2009)

Conclusion

1. Both $SrFeO_3$ and $BaFeO_3$ present helical spin order at ambient pressure resulting from the competing double exchange between conducting electron and superexchange between localized electron, though the wave vector in $BaFeO_3$ is shorter because of weakened double exchange resulting from larger lattice parameter.
2. Ferromagnetic phase transition will happen in both $SrFeO_3$ and $BaFeO_3$ under high pressure because of enhanced hybridization