NHSCP 2014@ISSP

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New Horizon of Strongly Correlated Physics

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ISSP, The University of Tokyo

Ab initio Studies on Mechanism for Iron-based Superconductors

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June 26, 2014, ISSP Kashiwa

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Outline

1. **Introduction**

   ***Ab initio* Approach**

2. **Orbital Selective Mottness, Magnetism**

3. **Phase Diagram, Superconducting Mechanism**

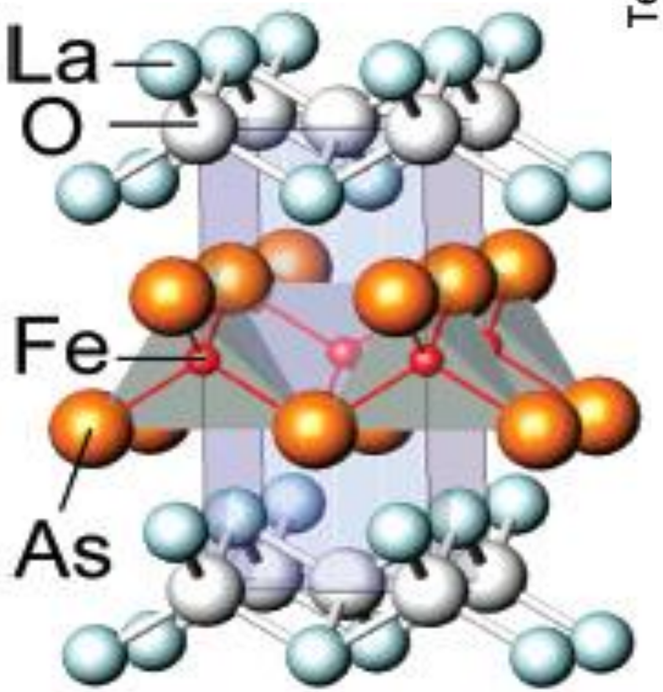
4. **Summary**

Introduction

Experimental Discovery

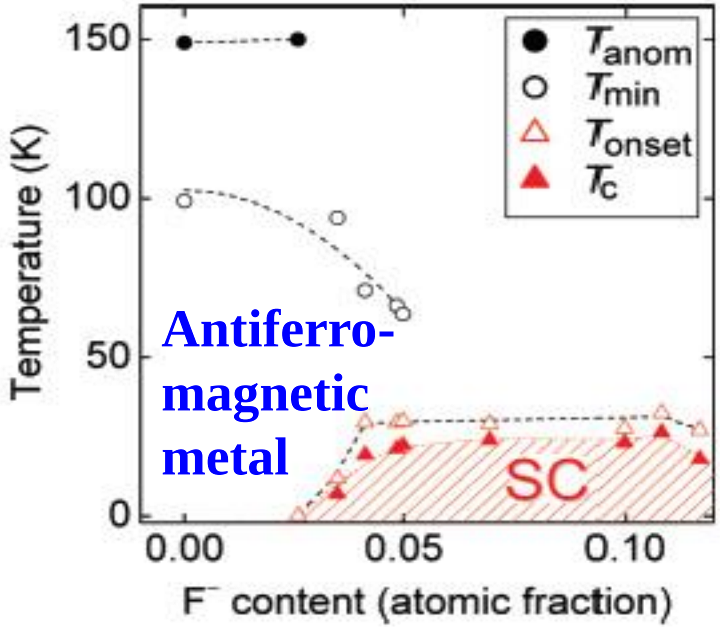
$LnFeAs(O_{1-x}F_x)$

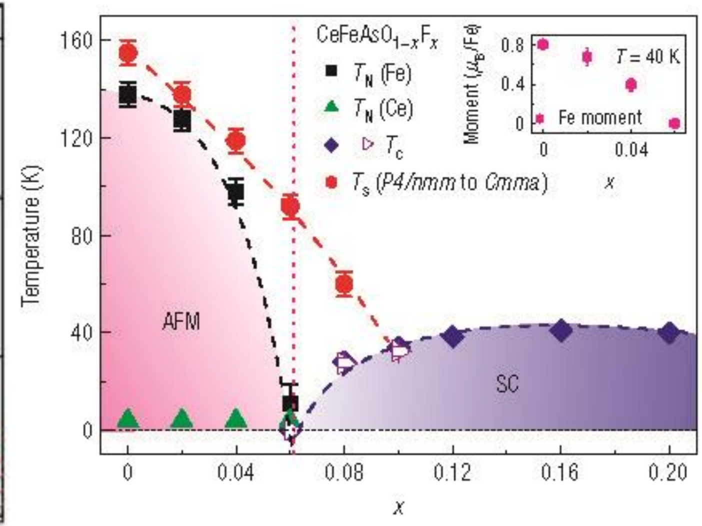
Ln = La, Pr, Sm, …



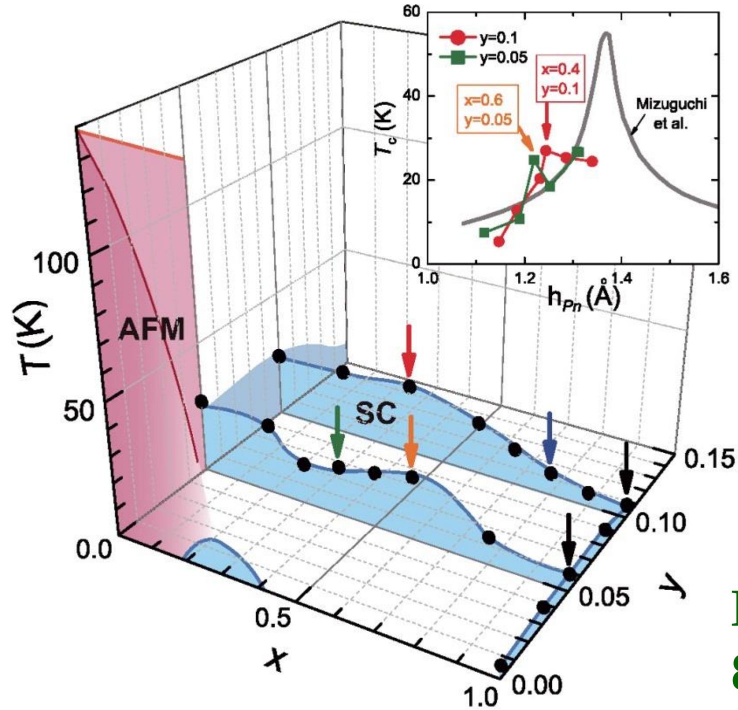
T_c ~ 26K-55K

Kamihara *et al*, JACS 130, 3296 (2008)





Zhao et al. Nat .Mat. 7,963 (2008)



Mukuda et al. PRB 89 (2013) 064511

DA

Global band structure

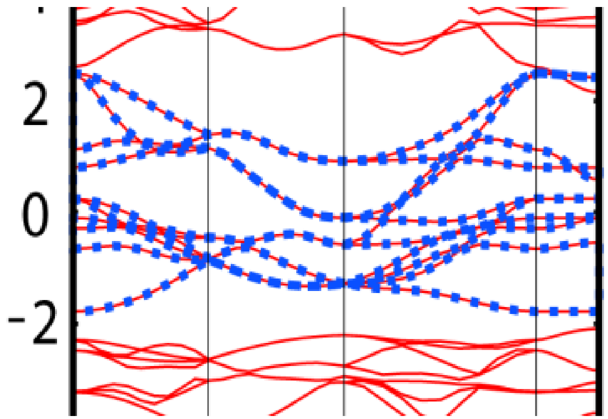
1111: LaFePO, LaFeAsO

122: $BaFe_2As_2$

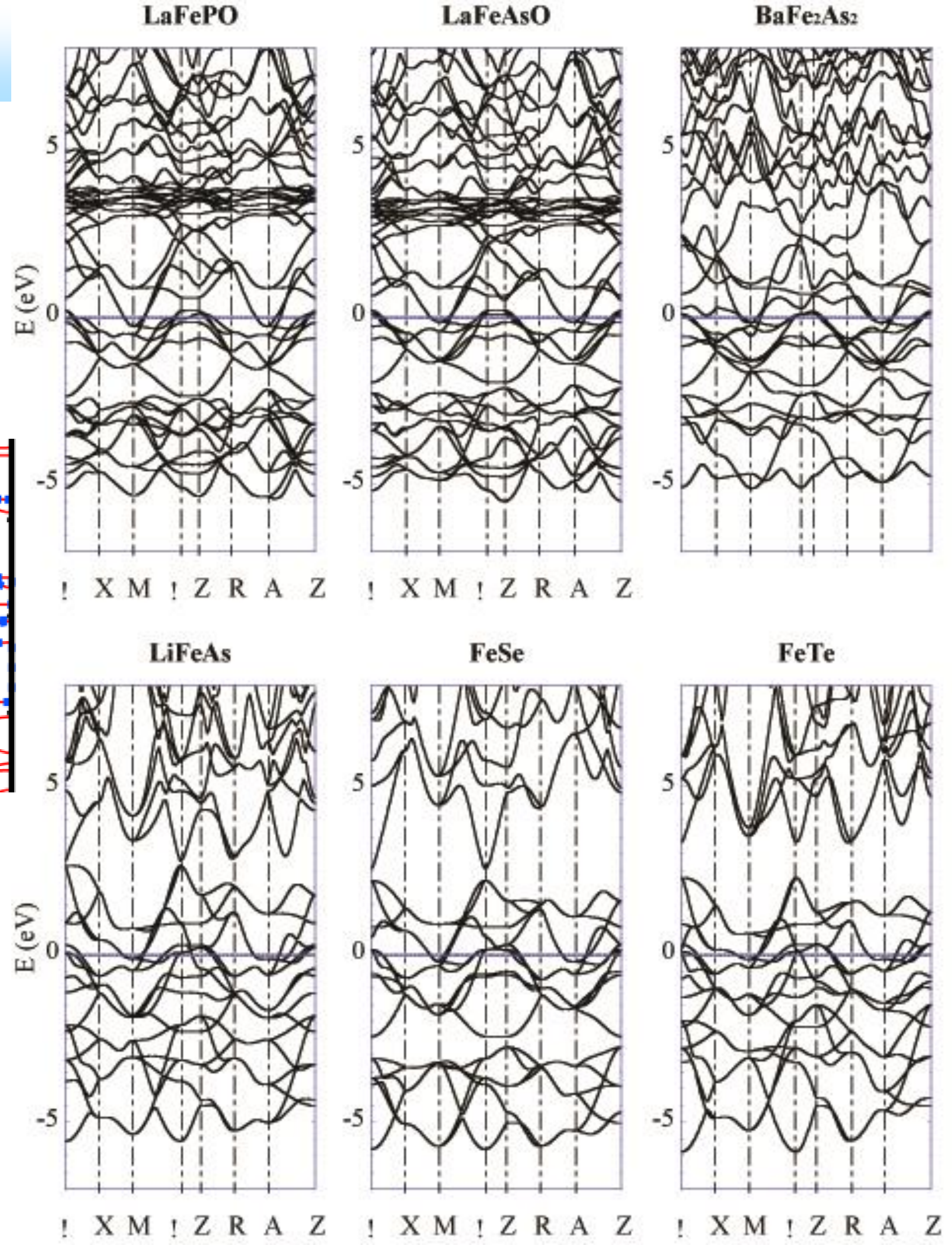
111: LiFeAs

11: FeSe, FeTe

Similar Fe 3*d* Bands



Bandwidth ~ 4.5 eV



Miyake, Nakamura, Arita, Imada
JPSJ 79 (2010) 044705

Diversity and strong family dependence

No AF order in LaFePO

Small AF ordered moment（0.36-0.83μ_B for LaFeAsO）

cf. LSDA overestimate the order (~2μ_B)

vs. large moment (2.25 μ_B for FeTe)

Variation of AF ordered pattern

(π,0) stripe in LaFeAsO vs. (π/2, π/2) bicollinear in FeTe

Role of electron correlation

Variation of T_c

Diversity cannot be explained by band strucuture

What controls the material dependence?

Bad metallic behavior

small Drude weight

Keimer *et al.* Timusk *et al.*

Chen *et al.*

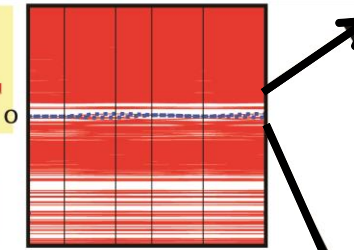
Unconventional T_1

First Principles Approach

downfolding;
Fe 3*d* 5 band models
(*d* model)

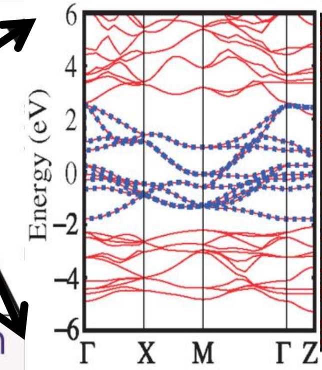
dimensional downfolding
→ 2 D effective model

1. Global electronic structure by DFT。



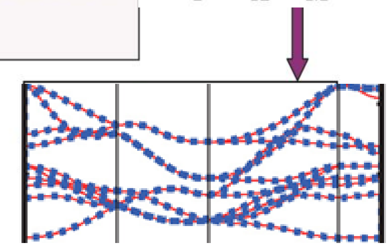
far from Fermi level

tens eV



2. downfolding

constrained RPA
(1) Screened Coulomb interaction
(2) Self-energy



target bands

Low-energy effective Hamiltonian

1/10-1/100 eV

3. Low-energy solver
variational Monte Carlo (VMC),
path-integral renormalization group (PIRG) ,
(cluster) dynamical mean-field theory (DMFT),
....

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int},$$
$$\mathcal{H}_0 = \sum_\sigma \sum_{i,j} \sum_{\nu,\mu} t_{i,j,\nu,\mu} c^\dagger_{i,\nu,\sigma} c_{j,\mu,\sigma},$$
$$\mathcal{H}_{\rm int} = \mathcal{H}_{\rm on-site} + \mathcal{H}_{\rm off-site}.$$

$$\mathcal{H}_{\rm on-site} = \frac{1}{2}\sum_{\sigma,\sigma'}\sum_i\sum_{\nu,\mu}\Big\{ U_{i,i,\mu,\nu} c^\dagger_{i,\nu,\sigma} c^\dagger_{i,\mu,\sigma'} c_{i,\mu,\sigma'} c_{i\nu,\sigma} + J_{i,i,\mu,\nu}\big(c^\dagger_{i,\nu,\sigma} c^\dagger_{i,\mu,\sigma'} c_{i,\nu,\sigma'} c_{i,\mu,\sigma} + c^\dagger_{i,\nu,\sigma} c^\dagger_{i,\nu,\sigma'} c_{i,\mu,\sigma'} c_{i,\mu,\sigma}\big)\Big\},$$

$$\mathcal{H}_{\rm off-site} = V_{nn} \sum_{\langle i,j\rangle,\nu,\mu} n_{i\nu} n_{j\mu} + V_{nnn} \sum_{\langle\langle k,l\rangle\rangle,\nu,\mu} n_{k\nu} n_{l\mu}$$

Review: Imada, Miyake:
J. Phys. Soc. Jpn. 79 (2010) 112001

Ab initio derivation of *U* by constrained RPA

	d model			dp/dpp model		
	$\bar{U}$ (eV)	$\bar{v}$ (eV)	$\bar{U}/\bar{v}$	$\bar{U}$ (eV)	$\bar{v}$ (eV)	$\bar{U}/\bar{v}$
LaFePO	2.47	14.15	0.174	4.13	18.96	0.218
LaFeAsO	2.53	14.85	0.171	4.23	19.46	0.217
$BaFe_2As_2$	2.80	15.59	0.180	5.24	20.38	0.257
LiFeAs	3.15	15.82	0.199	5.94	20.35	0.292
FeSe	4.24	17.53	0.242	7.21	21.37	0.337
FeTe	3.41	16.89	0.202	6.25	20.90	0.299

U / t **:*d* model**

LaFePO	**8**
LaFeAsO	**9**
FeTe	**11**
FeSe	**14**

smaller size of Wannier
⇒ larger bare Coulomb
smaller covalency
⇒ poor screening

Miyake, Nakamura, Arita, Imada
JPSJ 79 (2010) 044705

Variational Monte Carlo

Gros
Sorella *et al.*

Tahara, MI
JPSJ 77 (2008)
114701

$$|\psi\rangle = \mathcal{P}_{\rm J}\mathcal{P}^{\rm ex.}_{\rm d\text{-}h}\mathcal{P}_{\rm G}\,\mathcal{L}^{S=0}\,|\phi_{\rm pair}\rangle$$

$$|\phi_{\rm pair}\rangle = \left[\sum_{i,j} f_{ij}c^{\dagger}_{i\uparrow}c^{\dagger}_{j\downarrow}\right]^{N/2}|0\rangle$$

f_{ij} : pair-dependent variational parameter

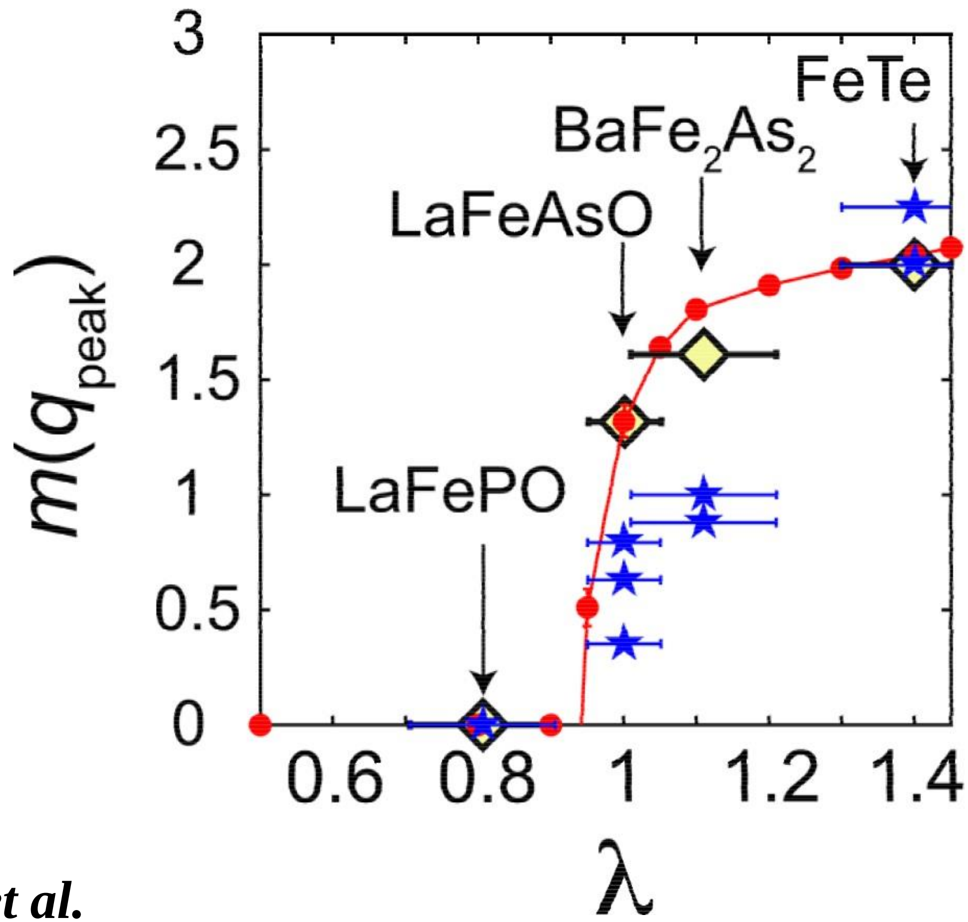
optimization of 1000-10000 variables to overcome bias

$$\mathcal{P}_{\rm G} = \exp\left[-g\sum_i n_{i\uparrow}n_{i\downarrow}\right]$$ **Gutzwiller factor**

$$\mathcal{L}^S = \frac{2S+1}{8\pi^2}\int d\Omega\, P_S(\cos\beta)\hat{R}(\Omega)$$ **quantum number projection**

Solution of low-energy solver

ordered magnetic moment



VMC result for *ab initio* models of mother compounds

★ experiment
◇ *ab initio* model
● λ scaled model

Misawa *et al.*
JPSJ 80 (2011) 023704
PRL 108 (2012) 177007

near magnetic quantum critical point

see also Yin Haule Kotliar Nat. Mat. (2011)

Detailed Study on Doping Effect

Orbital Selective Mottness and Charge Inhomogeneity

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Superconducting Mechanism

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Summary

1. ***Ab intio* electronic model shows s± superconducting phase by electron doping into stripe AF phase of LaFeAsO.**
   Agreement with experiment

2. **Orbital selective Mottness of $d_{X2\text{-}Y2}$ orbital holds an underlying key for the emergence of the high-T_c superconductivity.**
   Major role for both magnetism and superconductivity.

3. **Superconductivity emerges because of the charge instability accompanied by the PS caused by the strong 1st order AF/nematic transition.**
   Smoking gun is found in one-to-one correspondence between charge compressibility and superconductivity in various cases.

M. IMADA

Thank you