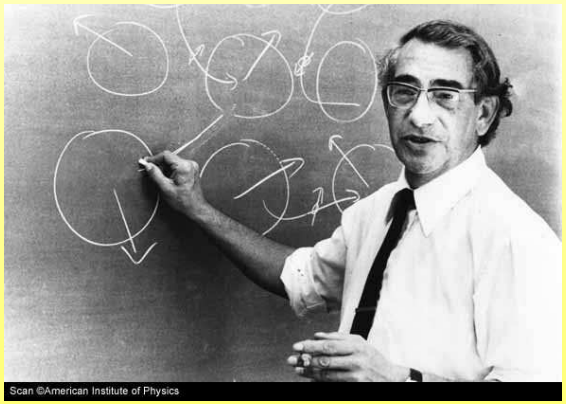
Hubbard and Hund from First Principles:



Dynamical Screening Effects in Iron Pnictide Compounds

Silke Biermann
Centre de Physique Théorique
Ecole Polytechnique, Palaiseau, France

The iron age of superconductivity ...

J|A|C|S
COMMUNICATIONS

Published on Web 02/23/2008

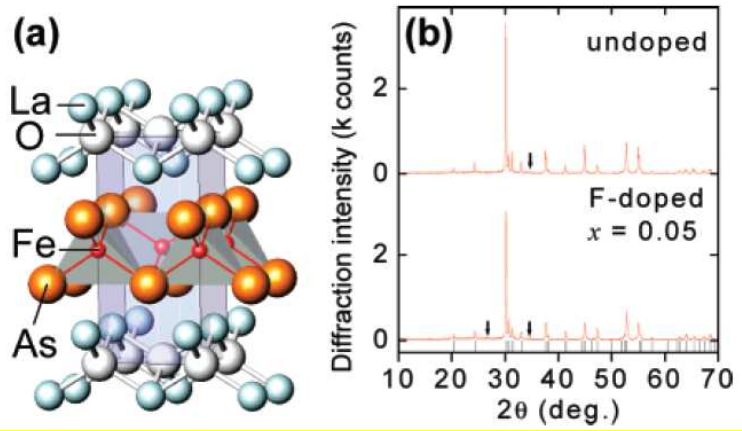
Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

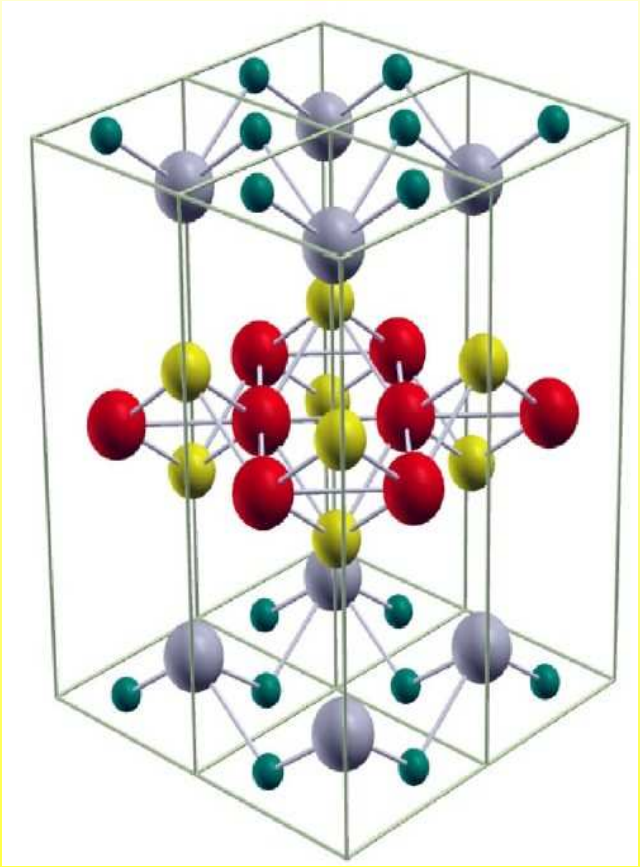
ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

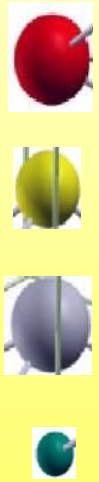
Received January 9, 2008; E-mail: hosono@msl.titech.ac.jp

Discovery of the copper-based superconductor $La_{2-x}Ba_xCuO_4$[1] with a high transition temperature (T_c) triggered extensive research with the intention of developing new transition-metal-based superconductors.[2,3] Currently, high T_c superconductors are limited to layered perovskites that contain CuO_2 structural units as the conduction layers. However, the T_c of the non-Cu-based superconductors in this category has remained low, although spin triplet superconductivity has been found in UPt_3 ($T_c \sim 0.54$ K)[4] and Sr_2RuO_4 ($T_c \sim 1.4$ K).[5,6] Here, we report a layered iron-based compound, LaOFeAs, which undergoes superconducting transition under doping with F^- ions at the O^{2-} site. Its T_c exhibits a



The “1111” family: LaFeAsO





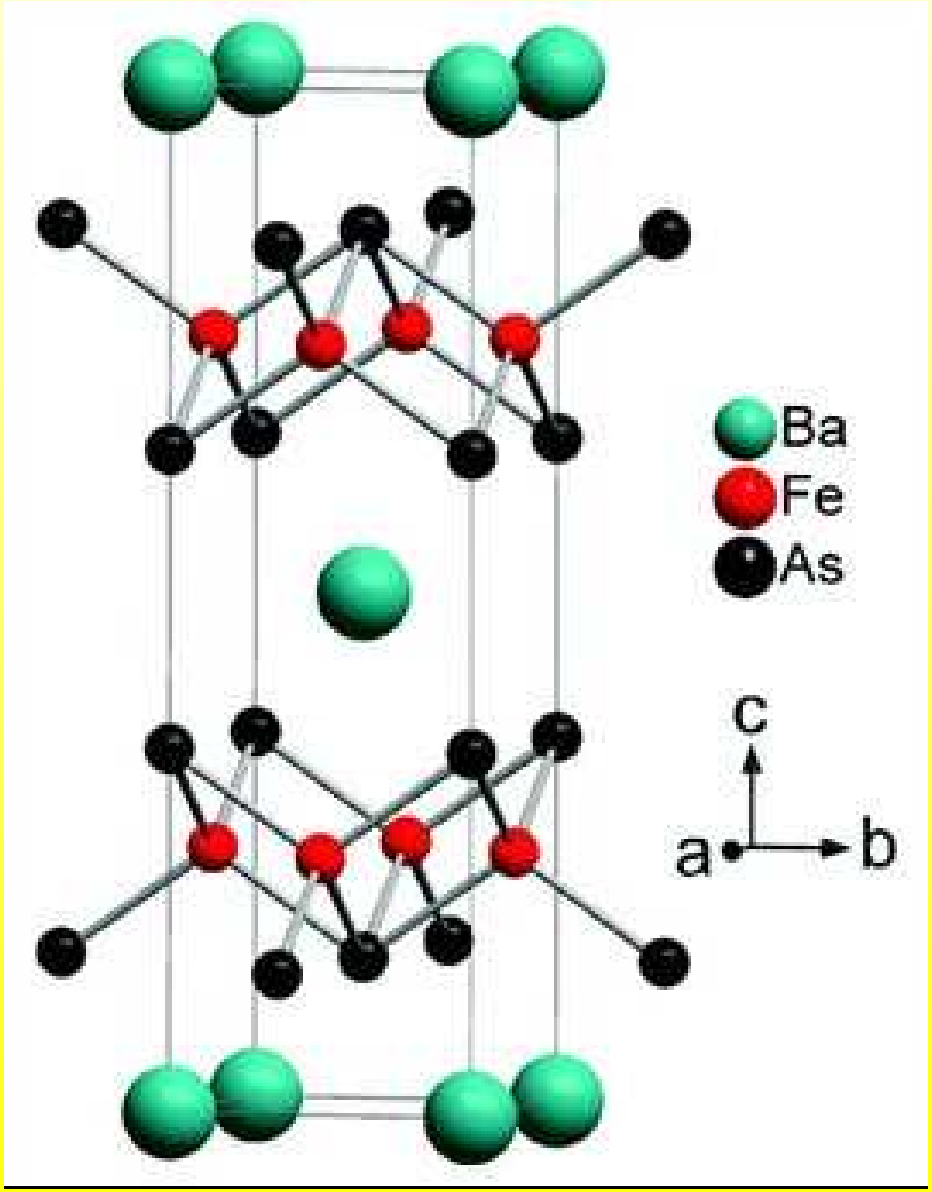
Fe

As

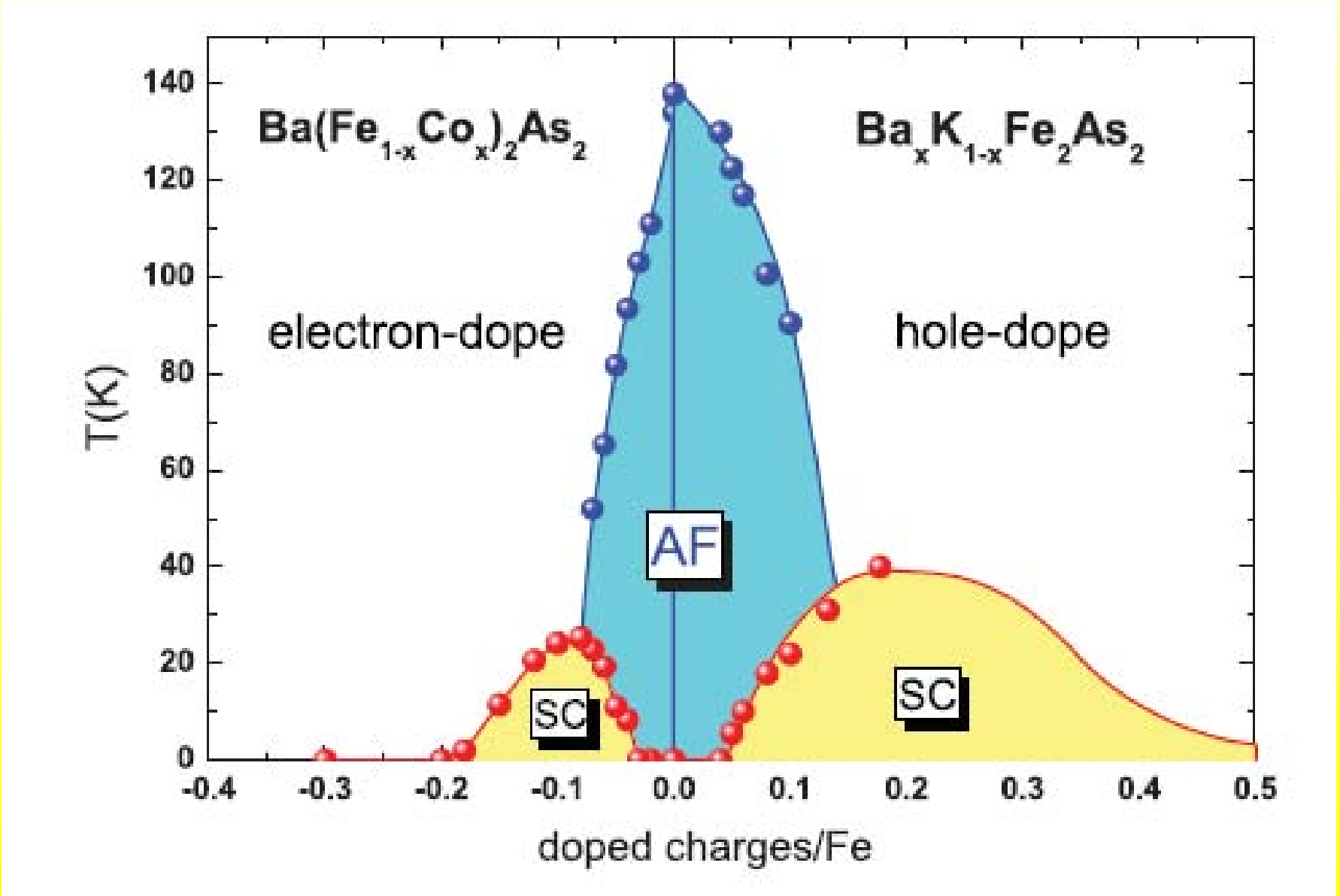
RE=La, Ce,
Pr, Sm,...

O

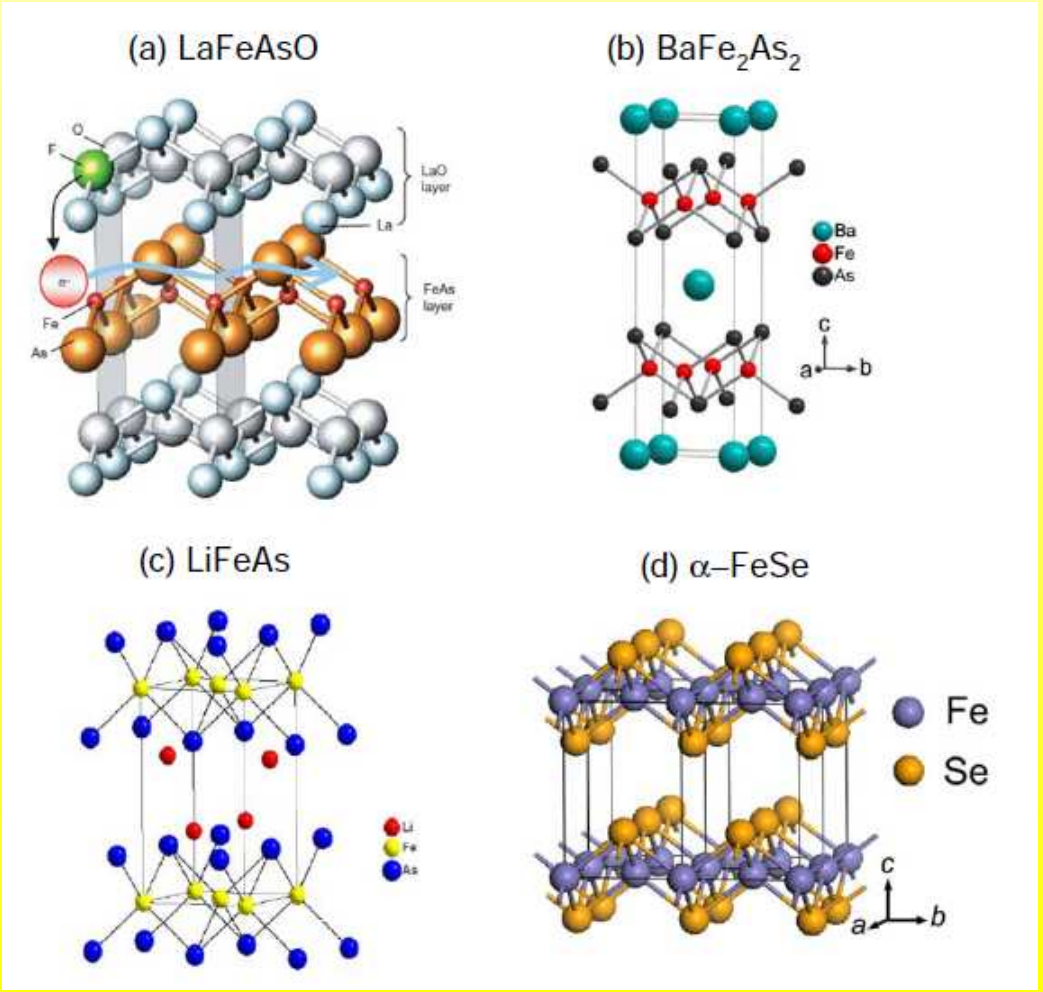
The “122” family: BaFe2As2

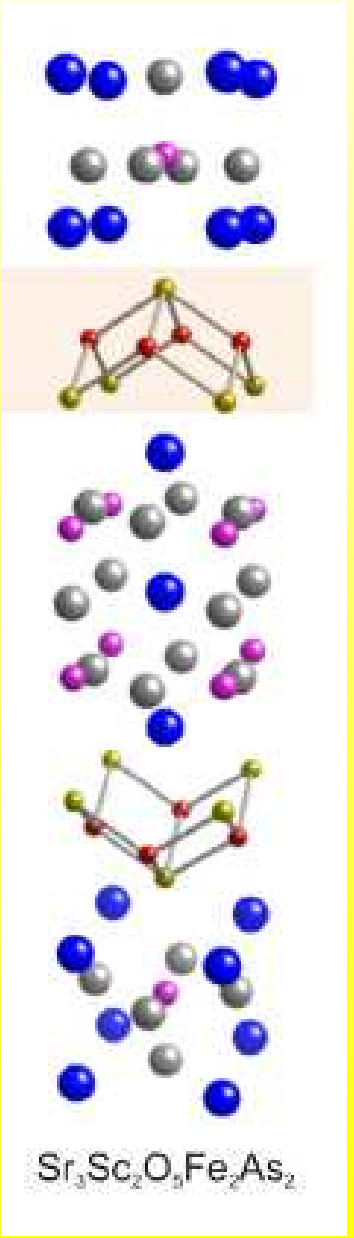


The “122” family: BaFe2As2



A zoo of compounds ...

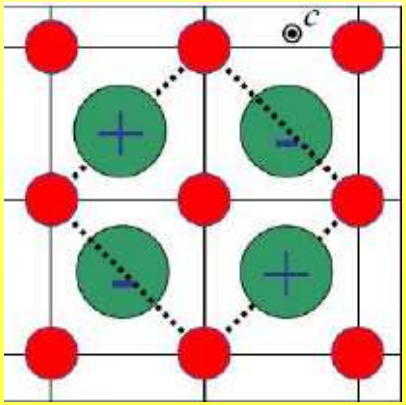




+ “245”

Features

- critical temperatures for superconductivity (under hole/electron-doping, pressure, substitutions ...) up to ~ 55 K
- near magnetic phases



- Fe forms a square lattice
- tetrahedral coordination
- near divalent Fe (d^6 configuration)

PRL 101, 026403 (2008) PHYSICAL REVIEW LETTERS week 11 JU

Is $LaFeAsO_{1-x}F_x$ an Electron-Phonon Superconductor?

L. Boeri,[1] O. V. Dolgov,[1] and A. A. Golubov[2]

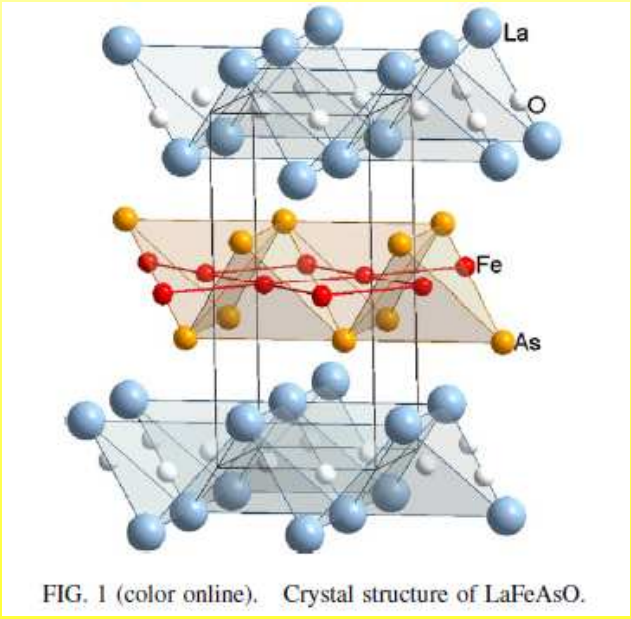
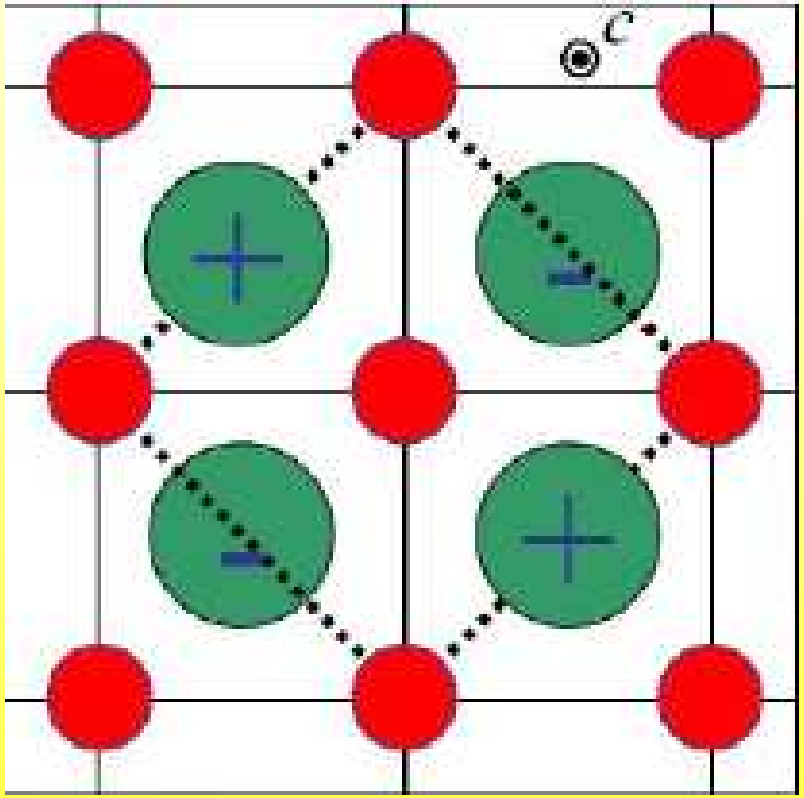


FIG. 1 (color online). Crystal structure of LaFeAsO.

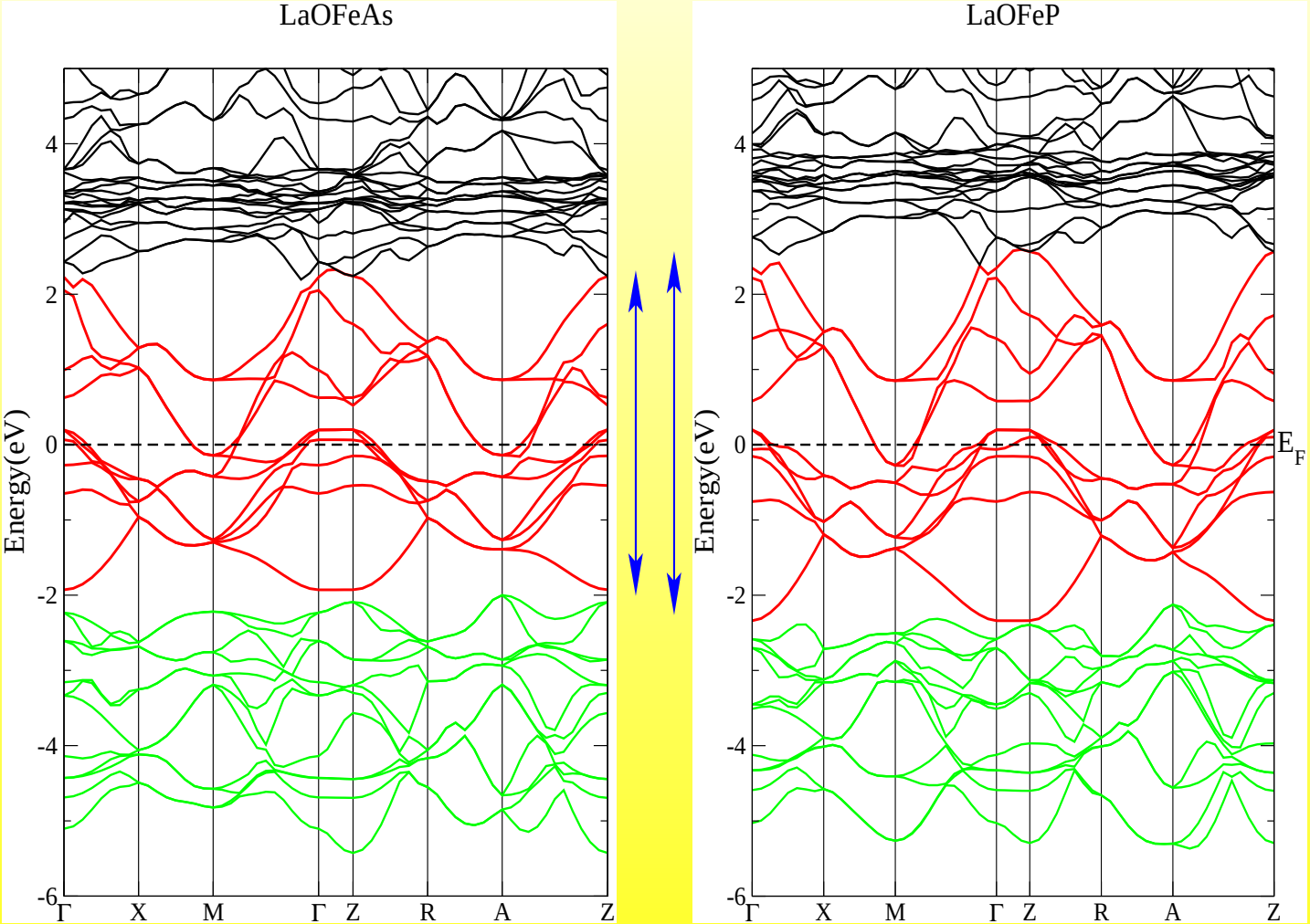
- Calculated T_C for phonon-mediated superconductivity: 0.8 K
- Experimental: 26 K
- Phonons cannot not account for superconductivity in this compound

Electronic structure



determined by Fe-As-plane: Fe 3d and As 4p states

LaFeAsO and LaFePO



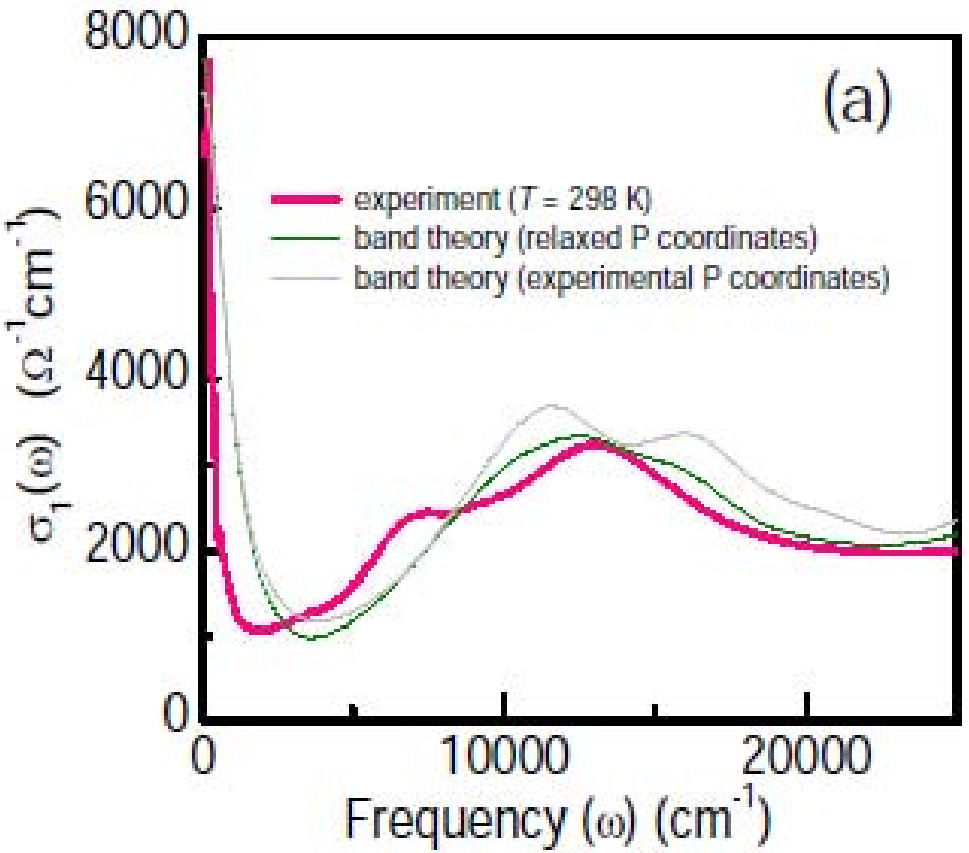
Fe-d states (red), hybridising with As-p and O-p bands (green)

Correlations in pnictides ?

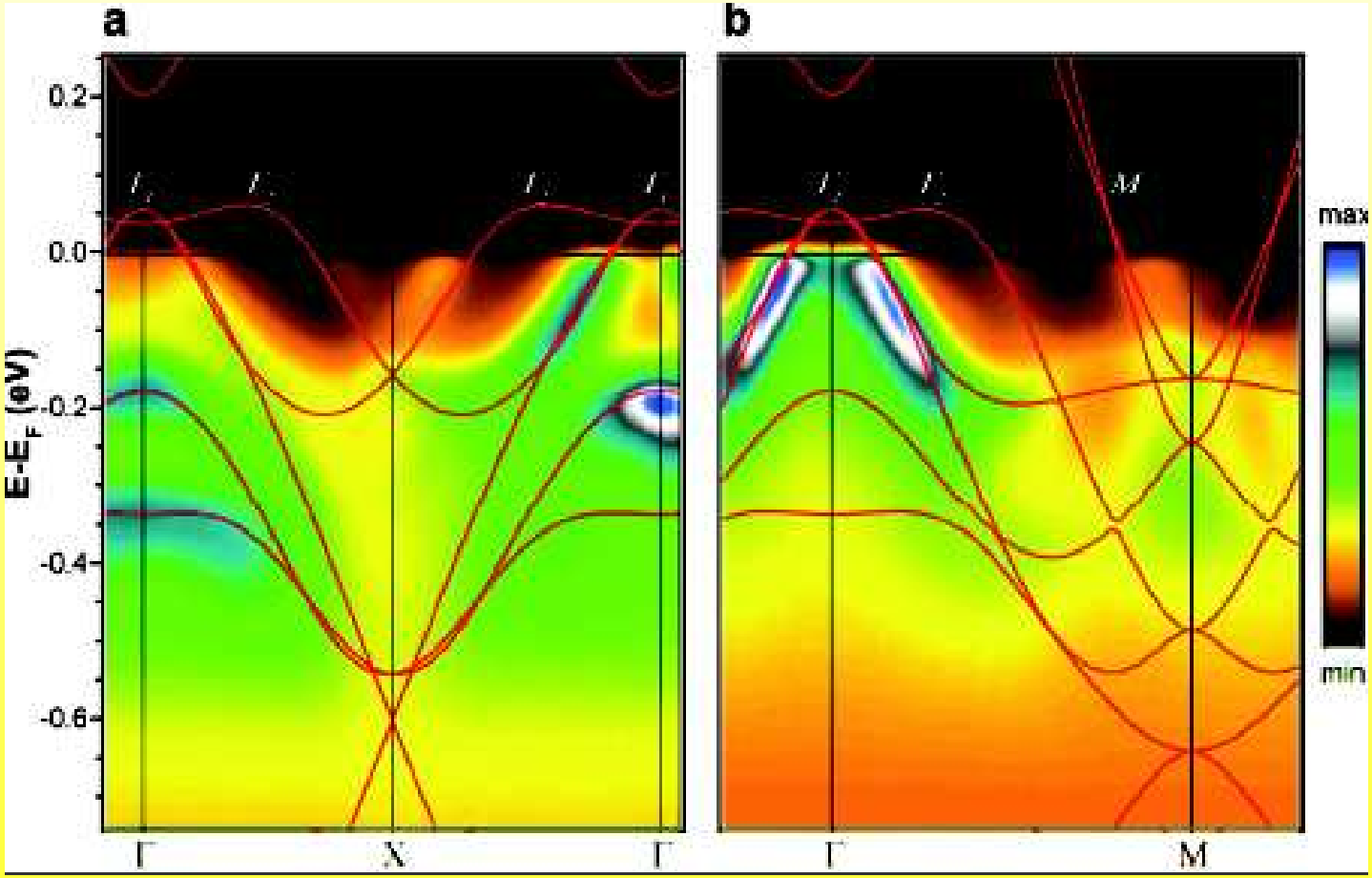
The example of LaFePO:

Electronic correlations in the iron pnictides

M. M. Qazilbash,[1,*], J. J. Hamlin,[1] R. E. Baumbach,[1] Lijun Zhang,[2] D. J. Singh,[2] M. B. Maple,[1] and D. N. Basov[1]
[1] *Physics Department, University of California-San Diego, La Jolla, California 92093, USA.*
[2] *Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA.*
(Dated: September 2, 2009)

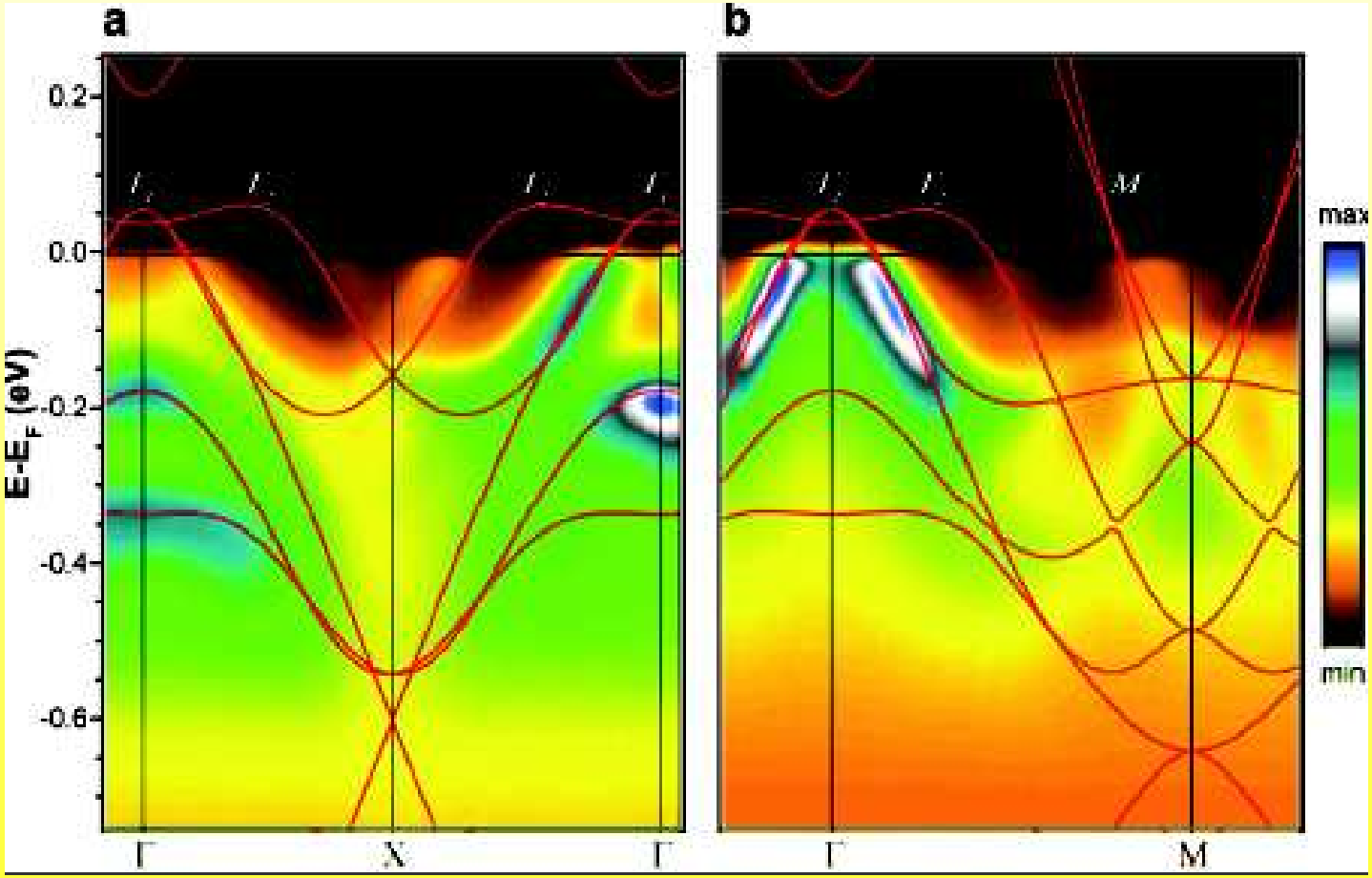


Correlations in pnictides ?



LaFePO: photoemission versus band structure
(Lu et al., 2008)

Correlations in pnictides ?



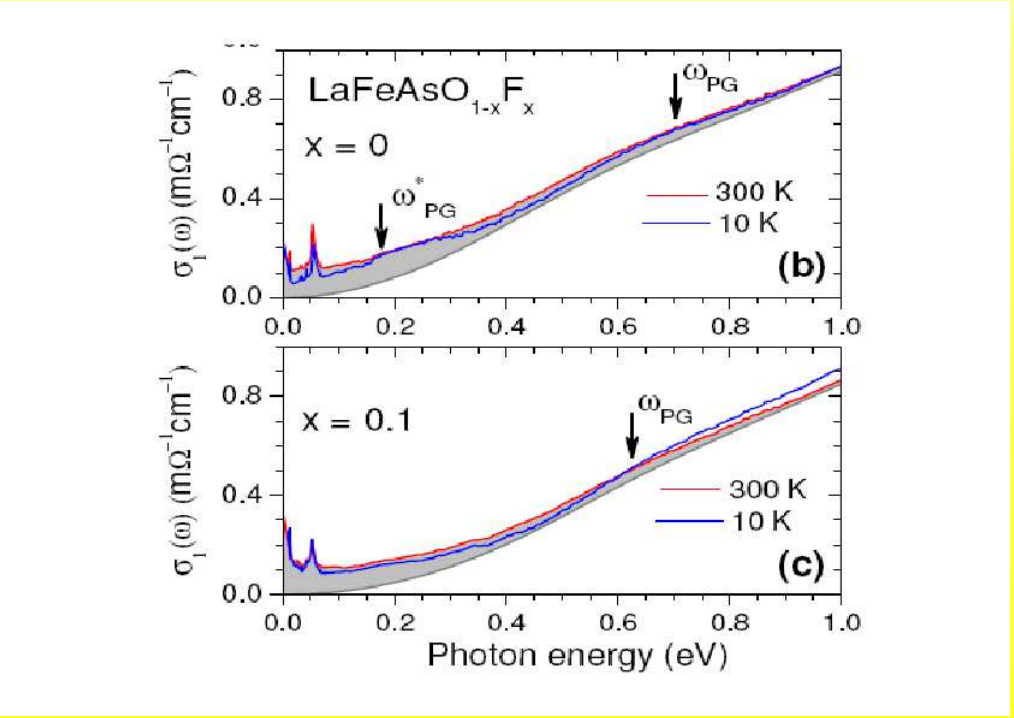
LaFePO: photoemission versus band structure
“after shifting the calculated bands up by 0.11 eV and then renormalizing by a factor 2.2” ...

Correlations in LaFeAsO?

Experimental (ARPES, XAS, optics ...) indications of moderate correlations

Mass enhancement from ARPES ~ 2

Optics (Boris et al.):



Dynamical Mean Field Calculations ...

PRL 100, 226402 (2008) PHYSICAL REVIEW LETTERS

Correlated Electronic Structure of $LaO_{1-x}F_xFeAs$

K. Haule, J. H. Shim, and G. Kotliar
Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA
(Received 9 March 2008; published 2 June 2008)

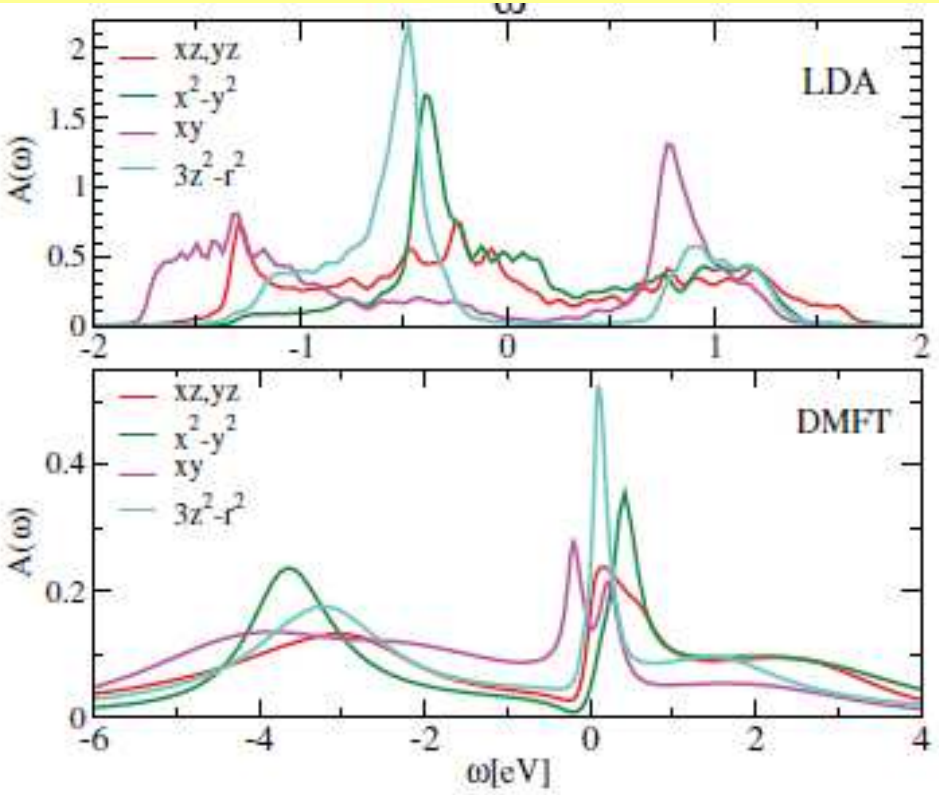


FIG. 3 (color). (a) DMFT density of states compared with LDA DOS. (b) Orbitally resolved Fe-3*d* density of states within

Close to Mott transition

Dynamical Mean Field Calculations ...

Coulomb Parameter U and Correlation Strength in LaFeAsO

V. I. Anisimov,[1] Dm. M. Korotin,[1] S. V. Streltsov,[1]
A. V. Kozhevnikov,[1,2] J. Kunes,[3] A. O. Shorikov,[1] and M. A. Korotin[1]

[1] *Institute of Metal Physics, Russian Academy of Sciences, 620041 Yekaterinburg GSP-170, Russia*
[2] *Joint Institute for Computational Sciences, Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831-6173, USA*
[3] *Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg 86135, Germany*

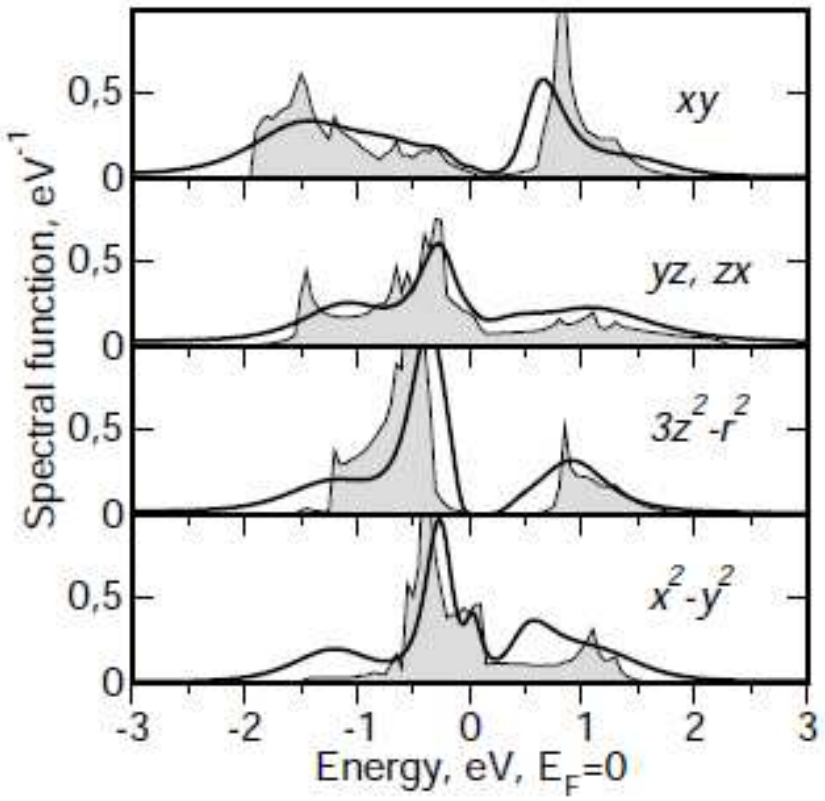


FIG. 3: Partial densities of states for different Fe-3d orbitals obtained within the DFT (filled areas) and LDA+DMFT or-

"LDA-like"

Multi-orbital Hamiltonian

$$H = \sum_{\{im\sigma\}} (H^{LDA}_{im,i'm'} - H^{double\ counting}_{im,i'm'}) a^{+}_{im\sigma} a_{i'm'\sigma}$$

$$+ \frac{1}{2} \sum_{imm'\sigma \text{ (correl. orb.)}} U^{i}_{mm'} n_{im\sigma} n_{im'-\sigma}$$

$$+ \frac{1}{2} \sum_{im \neq m'\sigma \text{ (correl. orb.)}} (U^{i}_{mm'} - J^{i}_{mm'}) n_{im\sigma} n_{im'\sigma}$$

- $H^{LDA}_{im,i'm'}$ calculated from density functional theory within the local density approximation (LDA)
- solved within dynamical mean field theory (DMFT)

$\rightarrow$ combined "LDA+DMFT" scheme

Anisimov et al., 1997, Lichtenstein et al., 1998

Parameters ...

Shim et al:

Hubbard U (= F_0) = 4 eV

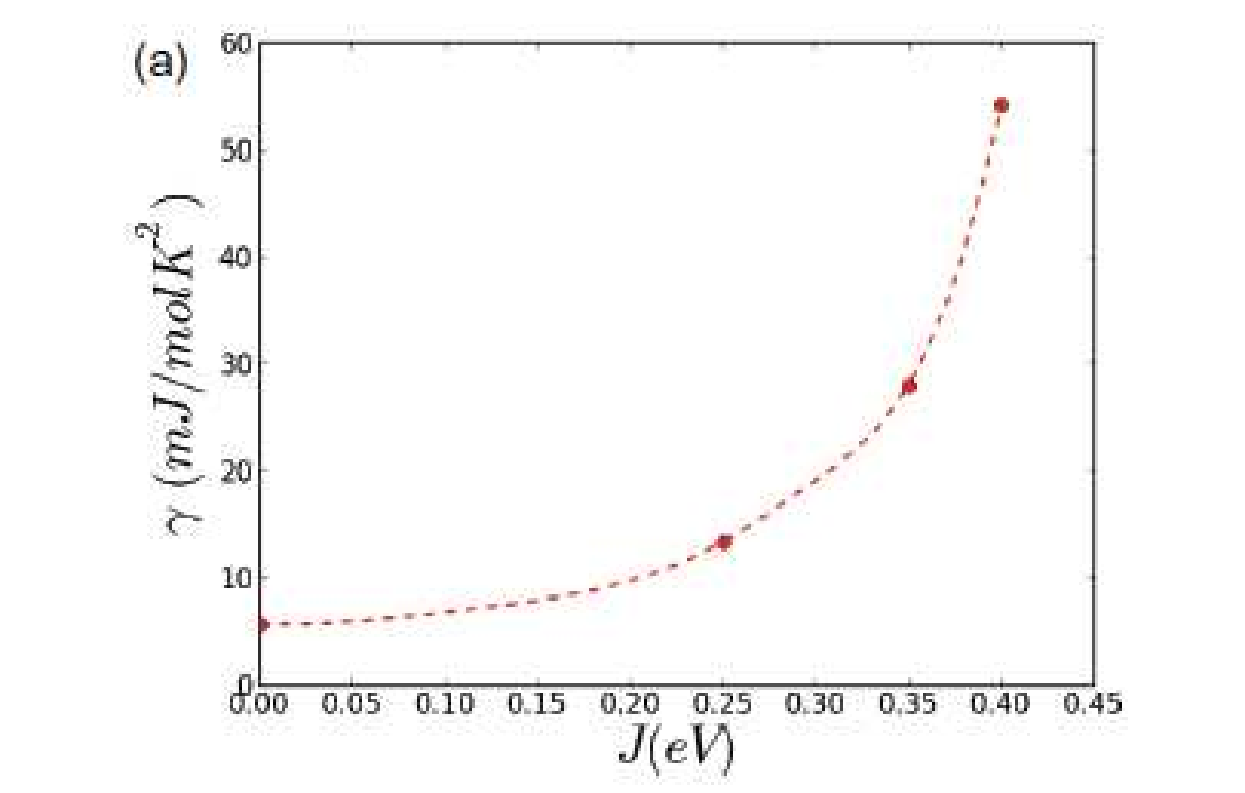
Hund's J = 0.7 eV

Anisimov et al:

Hubbard U (= F_0) = 0.8 eV

Hund's J = 0.5 eV

Sensitivity with respect to Hund's J



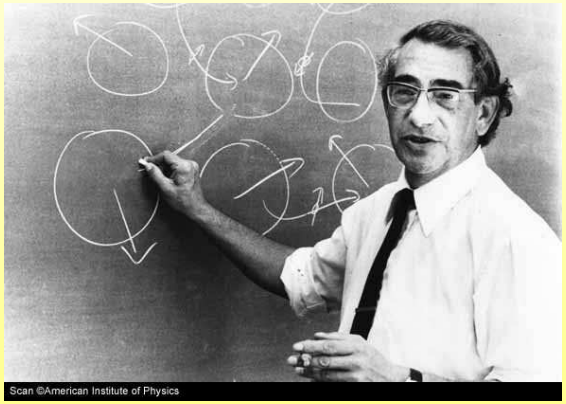
Haule et al., NJP 2009

Dynamical mean field calculations ...

... on iron pnictide compounds (1111, 122, 111, 11, ... (not exhaustive!)):

Haule et al. PRL 2008, New J. of Phys. (2009)
Craco et al., PRB 2008
Aichhorn et al., PRB 2009
Sangiovanni et al., PRL 2009
Han et al., PRL 2009
Anisimov et al. PRL 2009, Skornyakov et al. PRB 2009, PRL 2011
Laad et al., PRB 2009
Yee et al., PRB 2010
Ishida et al., PRB 2010, Liebsch PRB 2011
Yin et al. Nat. Mat. (2011)

Need for determination of ...



... Hubbard interaction U and Hund's coupling J from **first principles**

Bare interactions?

$$V_{m_1 m_2 m_3 m_4} \equiv \langle \phi_{m_1} \phi_{m_2} | \frac{1}{|r - r'|} | \phi_{m_3} \phi_{m_4} \rangle$$

$$= \iint d\boldsymbol{r} d\boldsymbol{r}' \phi^*_{m_1}(\boldsymbol{r}) \phi_{m_3}(\boldsymbol{r}) \frac{1}{|r - r'|} | \phi^*_{m_2}(\boldsymbol{r}') \phi_{m_4}(\boldsymbol{r}').$$

... calculate using Fe-3d Wannier functions

Bare interactions

LaFeAsO: ~ 20 eV

$$v^{\sigma\bar{\sigma}}_{mm'}|_{\mathrm{cRPA}} = \begin{pmatrix} 20.54 & 18.98 & 18.23 & 18.66 & 18.66 \\ 18.98 & 20.89 & 19.25 & 18.66 & 18.66 \\ 18.23 & 19.25 & 19.22 & 17.93 & 17.93 \\ 18.93 & 18.66 & 17.93 & 19.36 & 17.96 \\ 18.93 & 18.66 & 17.93 & 17.96 & 19.36 \end{pmatrix}.$$

$$v^{\sigma\sigma}_{mm'}|_{\mathrm{cRPA}} = \begin{pmatrix} 0 & 18.11 & 17.41 & 18.43 & 18.43 \\ 18.11 & 0 & 18.86 & 17.93 & 17.93 \\ 17.41 & 18.86 & 0 & 17.23 & 17.23 \\ 18.43 & 17.93 & 17.23 & 0 & 17.28 \\ 18.43 & 17.93 & 17.23 & 17.28 & 0 \end{pmatrix}$$

(L. Vaugier et al., unpublished)

Parametrisation

$$V_{m_1 m_2 m_1 m_2} = \langle \phi_{m_1} \phi_{m_2} | \frac{1}{|r - r'|} | \phi_{m_1} \phi_{m_2} \rangle = \sum_k a_k F^{(k)}$$

with the Slater integrals $V \equiv F^{(k)}$.
For 3d-electrons:

$$\begin{aligned} U &= F^{(0)} \\ J &= \frac{1}{14} \left(F^{(2)} + F^{(4)} \right) \\ \frac{F^{(4)}}{F^{(2)}} &\sim 0.625 \end{aligned} \qquad (1)$$

Screened interactions?

$$W_{m_1 m_2 m_3 m_4}(\omega) \equiv \langle \phi_{m_1} \phi_{m_2} | \epsilon^{-1}(\omega) \frac{1}{|r - r'|} | \phi_{m_3} \phi_{m_4} \rangle$$

Partially Screened interactions?

$$U_{m_1 m_2 m_3 m_4}(\omega) \equiv \langle \phi_{m_1} \phi_{m_2} | \epsilon_r^{-1}(\omega) \frac{1}{|r - r'|} | \phi_{m_3} \phi_{m_4} \rangle$$

with a “partial dielectric function” $\epsilon_r^{-1}(\omega)$ that includes screening processes not included in the low-energy Hamiltonian

What's U in a solid?

... an answer from RPA:

Divide $P = P_d + P_r$ where P_d = polarization of the correlated orbitals (e.g. 3d orbitals)
Then:

$$\begin{aligned} W &= [1 - vP]^{-1} v \\ &= [1 - W_r P_d]^{-1} W_r \end{aligned}$$

where W_r that does not include 3d-3d screening:

$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$

Identify $U = \langle | W_r(\omega = 0) | \rangle$!

F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S.B., A. I. Lichtenstein PRB **70** *195104 (2004)*

L. Vaugier, PhD thesis (2011) & L. Vaugier, H. Jiang, SB, to be published

Remarks

$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$

$$U = \langle \phi\phi | W_r(0) | \phi\phi \rangle$$

- More generally: $U = U(\omega)$
- U depends on model (non-interacting Hamiltonian and choice of correlated orbitals)

$\rightarrow$ choice of
(i) screening processes to be cut out from P_d
(ii) orbitals for matrix elements

Hund's coupling

Matrix form

$$J_{m_1 m_2} \equiv \langle \phi_{m_1} \phi_{m_2} | \epsilon_r^{-1}(\omega) \frac{1}{|r - r'|} | \phi_{m_2} \phi_{m_1} \rangle$$

Slater parametrisation:

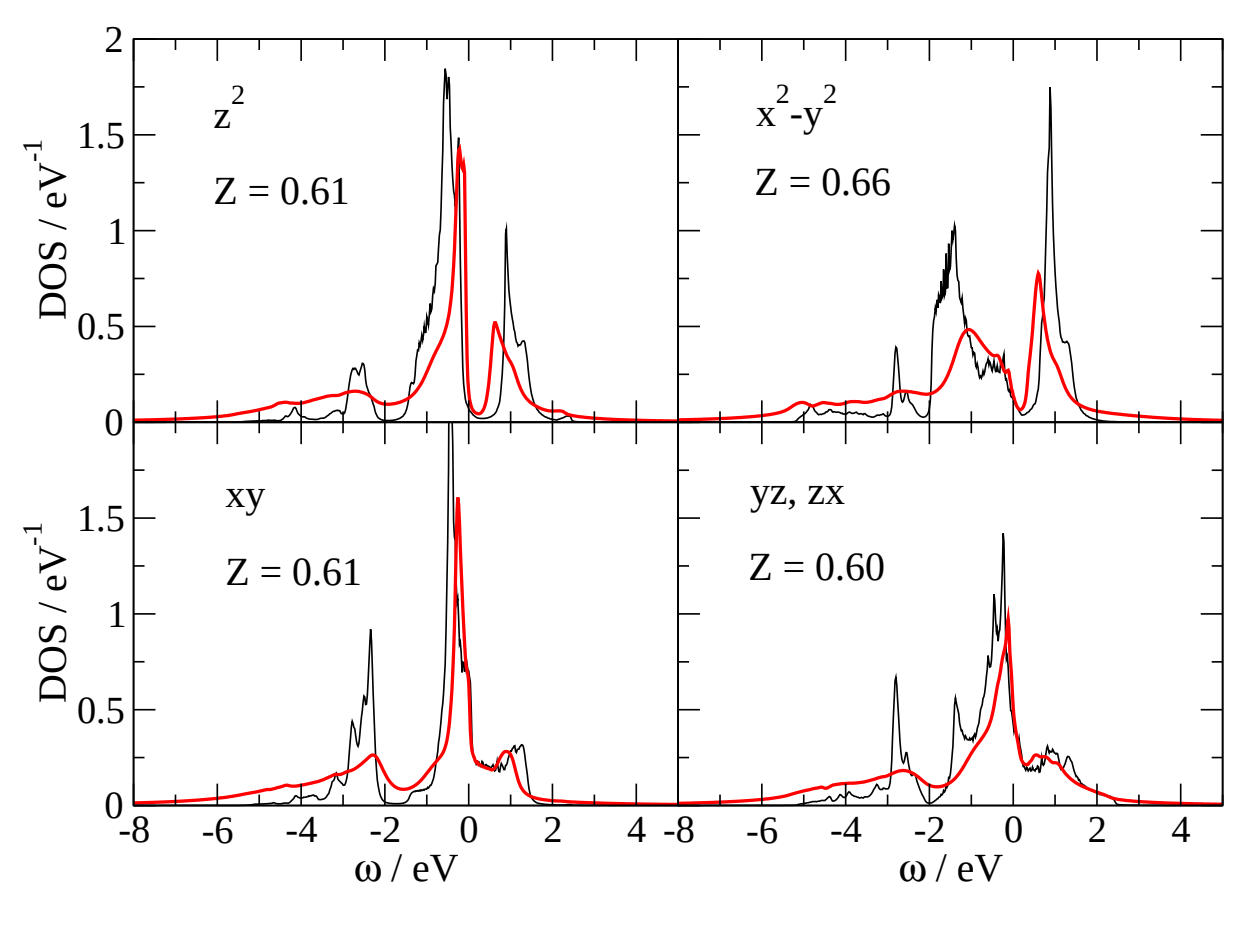
$$J = \frac{1}{14} \left(F^{(2)} + F^{(4)} \right)$$

Hubbard and Hund in pnictides

- Screening of U $\rightarrow$ one order of magnitude
- J weakly screened
- Variations between different compounds

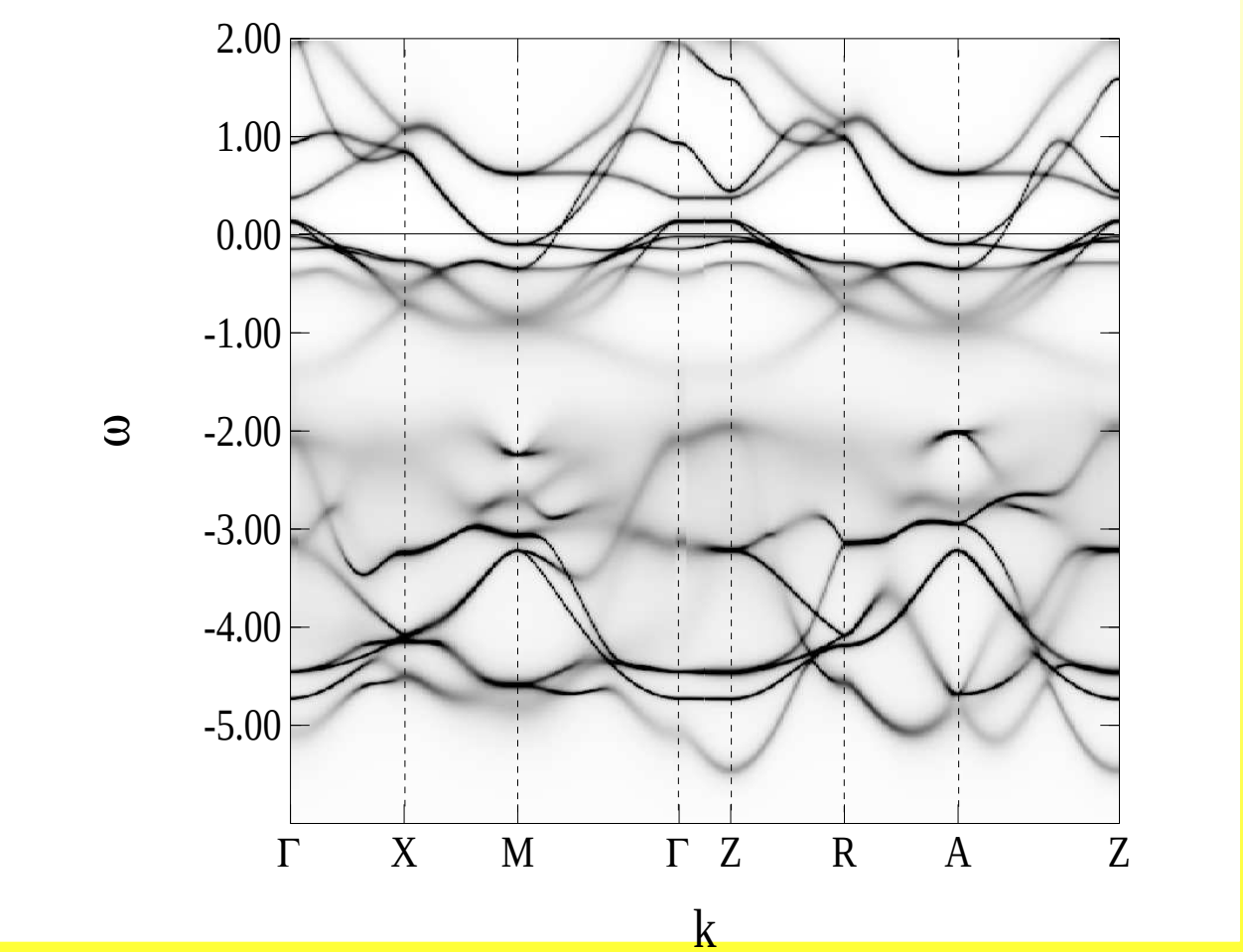
(L. Vaugier, H. Jiang, SB, to be published)

LaFeAsO in DMFT



Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges, SB, PRB 2009

LaFeAsO in DMFT



Well-defined quasi-particles close to E_F, damping effects beyond ~ 0.5 eV.

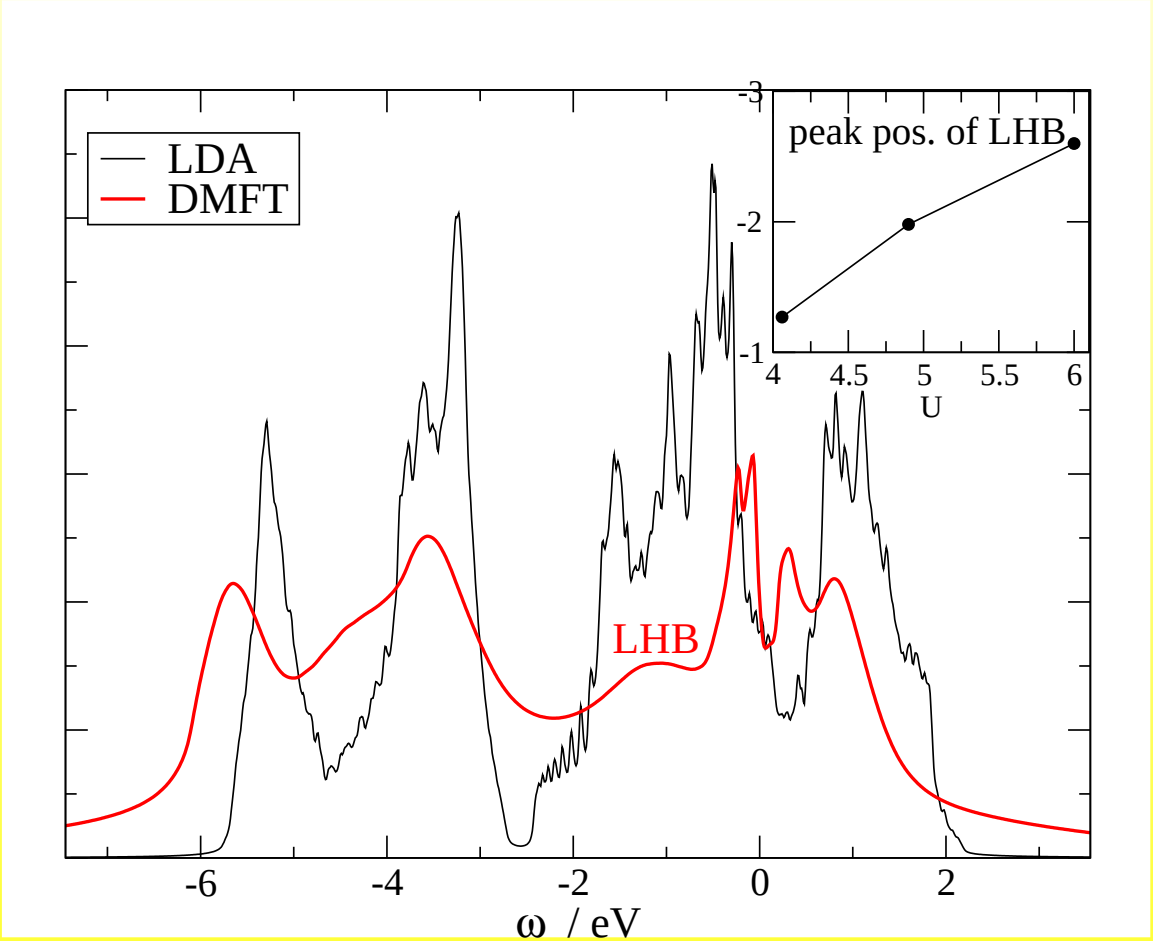
Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges, SB, PRB 2009

FeSe

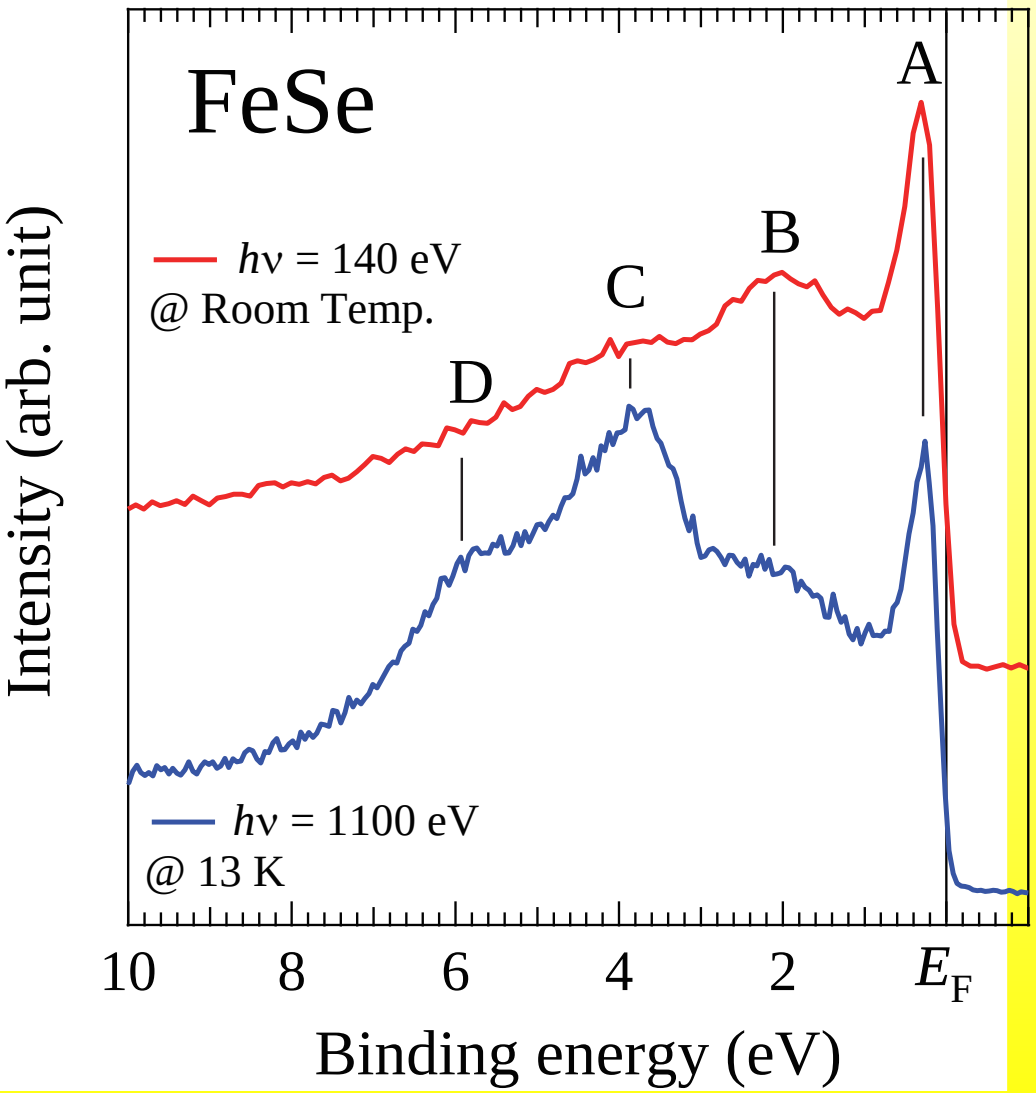
Using this same (CRPA-) procedure for FeSe yields:
U=4.06 eV, J=0.91 eV
$\rightarrow$ *Stronger correlations?*

Cf ARPES for Te-doped FeSe claims to see effective mass enhancements up to 23 !
(Tamai et al, arXiv 12/2009)

FeSe



Hubbard band?
Aichhorn, SB, Miyake, Georges, Imada, PRB 2010.



Yoshida et al, JPSJ 2009.

FeSe

PHYSICAL REVIEW B **82**, 184511 (2010)

Electron correlation in the FeSe superconductor studied by bulk-sensitive photoemission spectroscopy

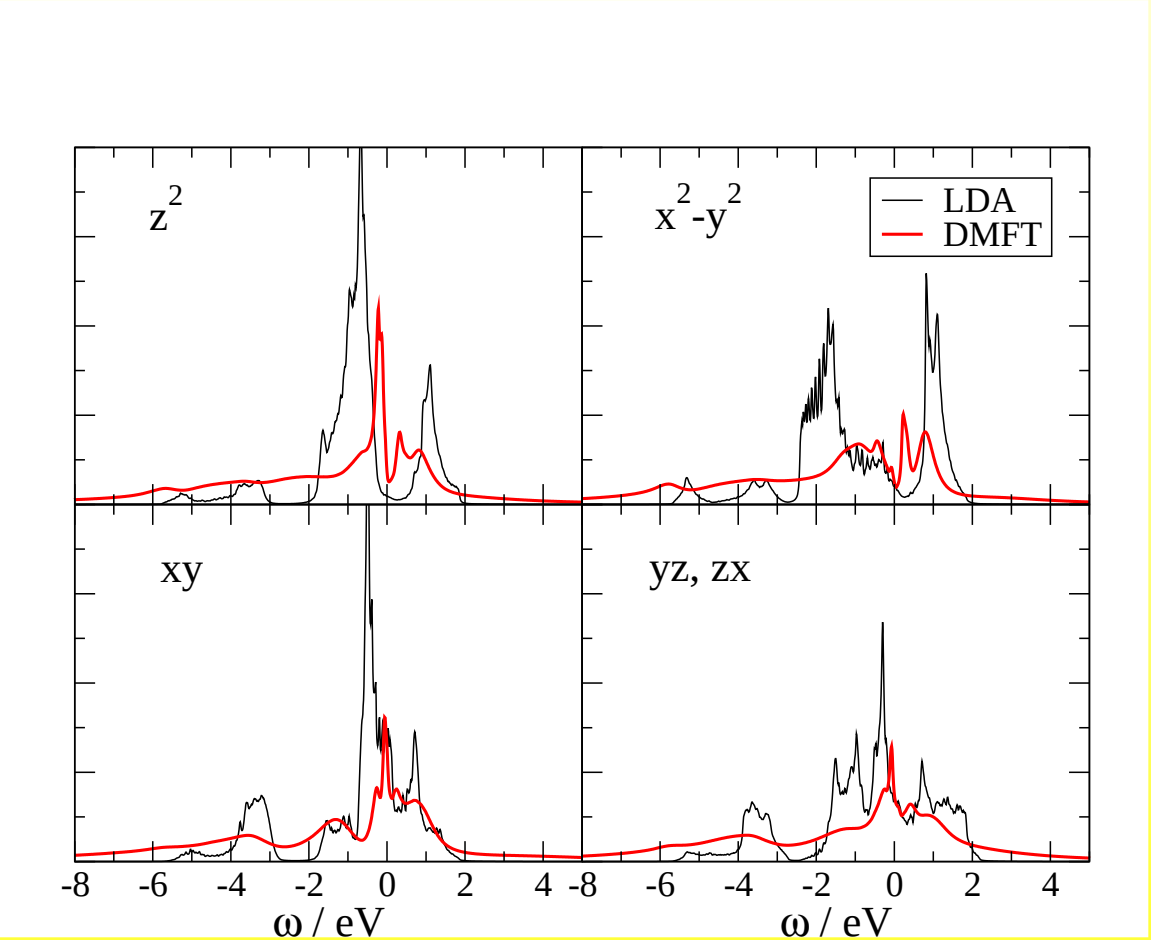
A. Yamasaki,[1] Y. Matsui,[1] S. Imada,[2] K. Takase,[3] H. Azuma,[3] T. Muro,[4] Y. Kato,[4,*] A. Higashiya,[5,†] A. Sekiyama,[6] S. Suga,[6] M. Yabashi,[4] K. Tamasaku,[5] T. Ishikawa,[5] K. Terashima,[2] H. Kobori,[1] A. Sugimura,[1] N. Umeyama,[7,8] H. Sato,[9] Y. Hara,[10] N. Miyagawa,[7] and S. I. Ikeda[8]

.....

FeSe. The self-energy correction provides the larger mass enhancement value ($Z^{-1}=3.6$) than in Fe-As superconductors and enables us to separate an incoherent part from the spectrum. These features are quite consistent with the results of recent dynamical mean-field calculations, in which the incoherent part is attributed to the lower Hubbard band.

Hubbard band!

FeSe



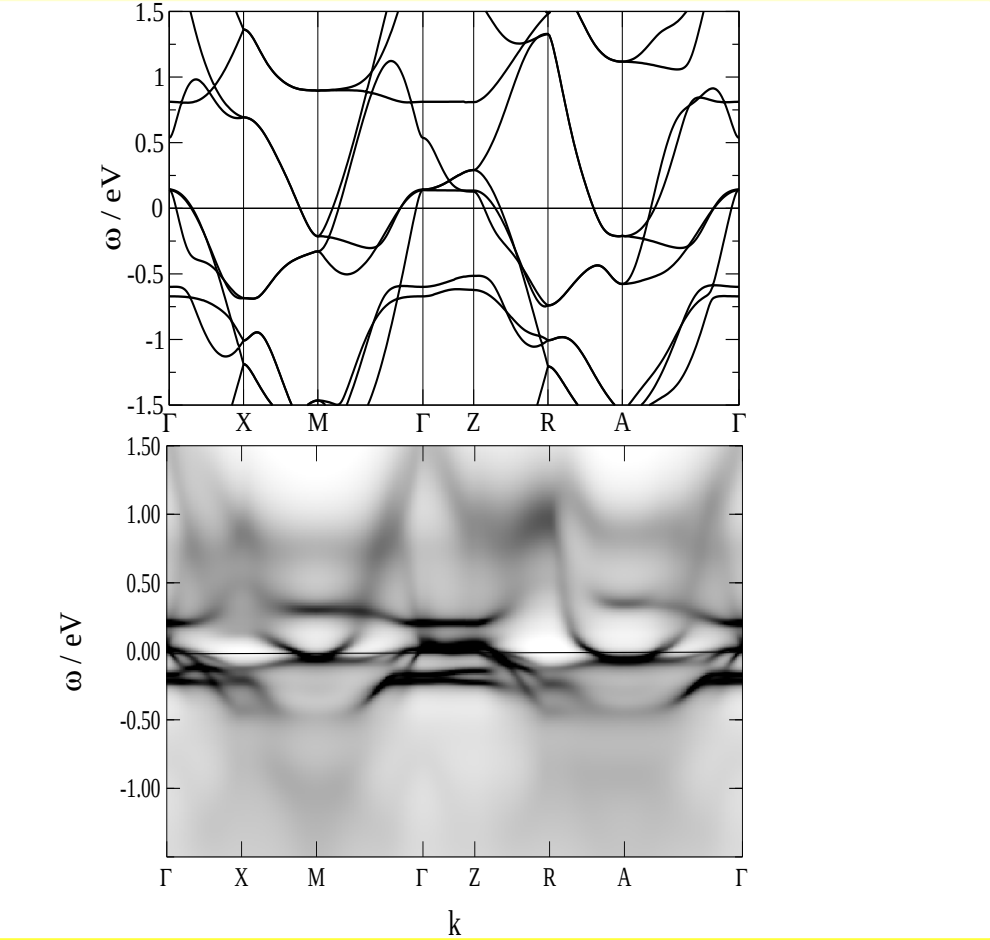
effective masses: ~ 2 for $x^2 - y^2$, ~ 5 for xy

But: large quasi-particle (?) damping

$(-\mathrm{Im}\Sigma(i0^+)_{xy} \simeq 0.2\,\mathrm{eV}$)

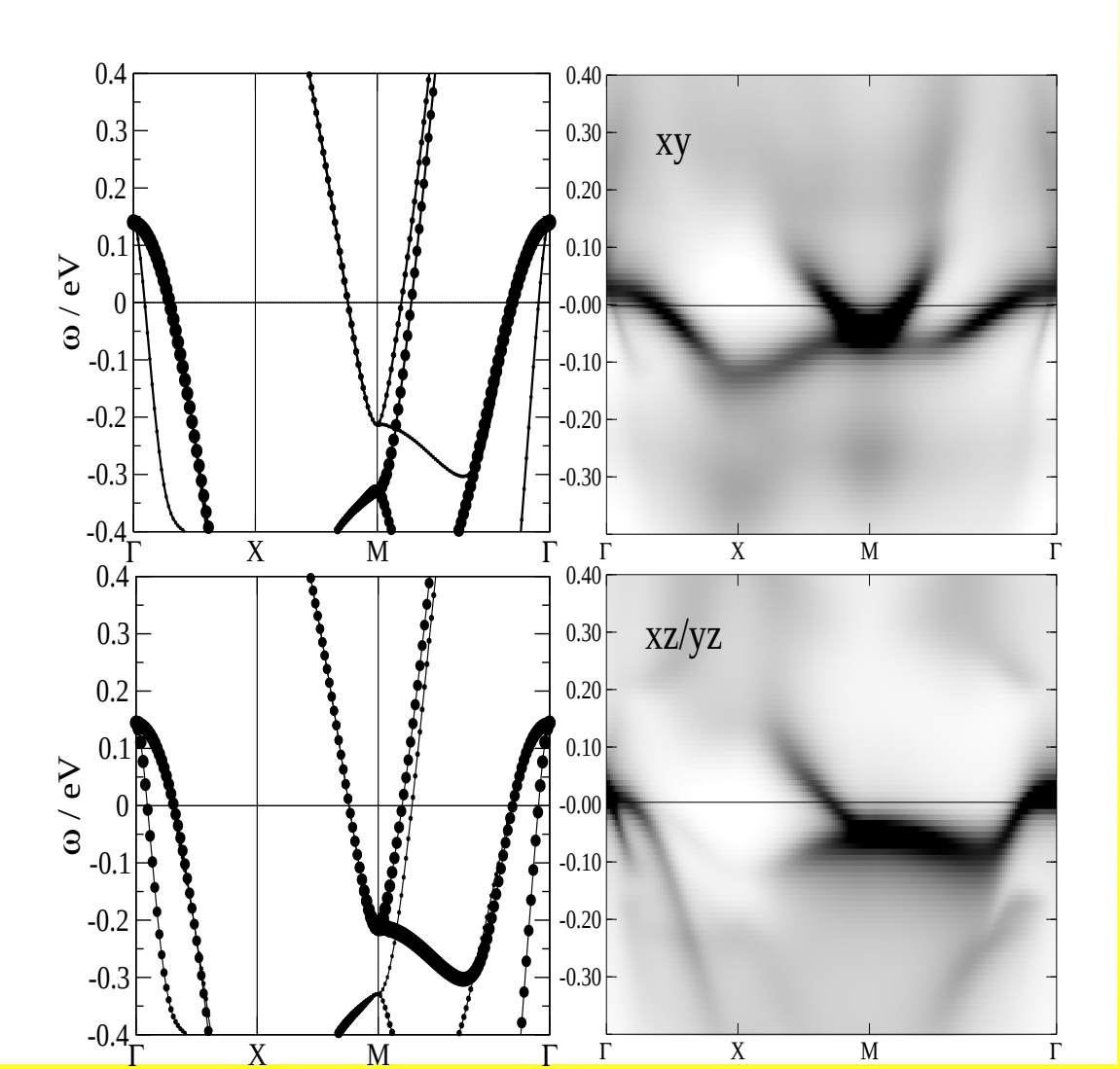
very bad metal !

FeSe: bands & spectral function



effective masses: ~ 2 for $x^2 - y^2$, ~ 5 for xy

FeSe: spectral function



crystal field shifts make direct extraction of mass enhancements from PES difficult !

What's U in a solid?

... an answer from RPA:

Divide $P = P_d + P_r$ where P_d = polarization of the correlated orbitals (e.g. 3d orbitals)
Then:

$$\begin{aligned} W &= [1 - vP]^{-1} v \\ &= [1 - W_r P_d]^{-1} W_r \end{aligned}$$

where W_r that does not include 3d-3d screening:

$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$

Identify $U = \langle | W_r(\omega = 0) | \rangle$!

F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S.B., A. I. Lichtenstein PRB **70** *195104 (2004)*

L. Vaugier, PhD thesis (2011) & L. Vaugier, H. Jiang, SB, to be published

What's U in a solid?

... an answer from RPA:

Divide $P = P_d + P_r$ where P_d = polarization of the correlated orbitals (e.g. 3d orbitals)
Then:

$$\begin{aligned} W &= [1 - vP]^{-1} v \\ &= [1 - W_r P_d]^{-1} W_r \end{aligned}$$

where W_r that does not include 3d-3d screening:

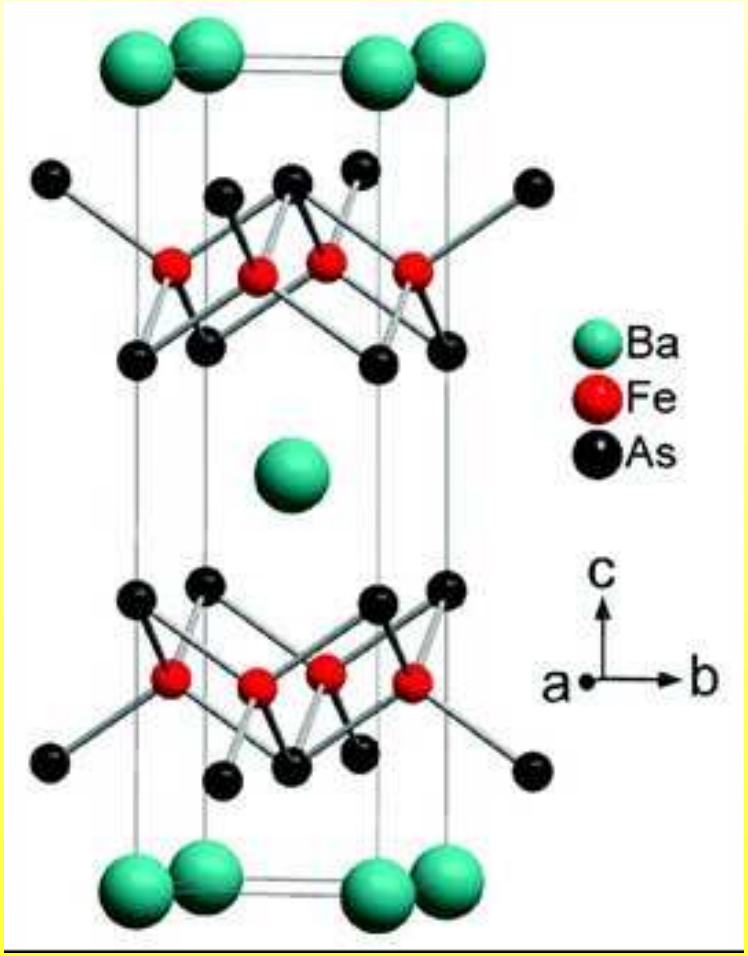
$$W_r(\omega) = [1 - vP_r(\omega)]^{-1} v$$

Identify $U(\omega) = \langle |W_r(\omega)| \rangle$!

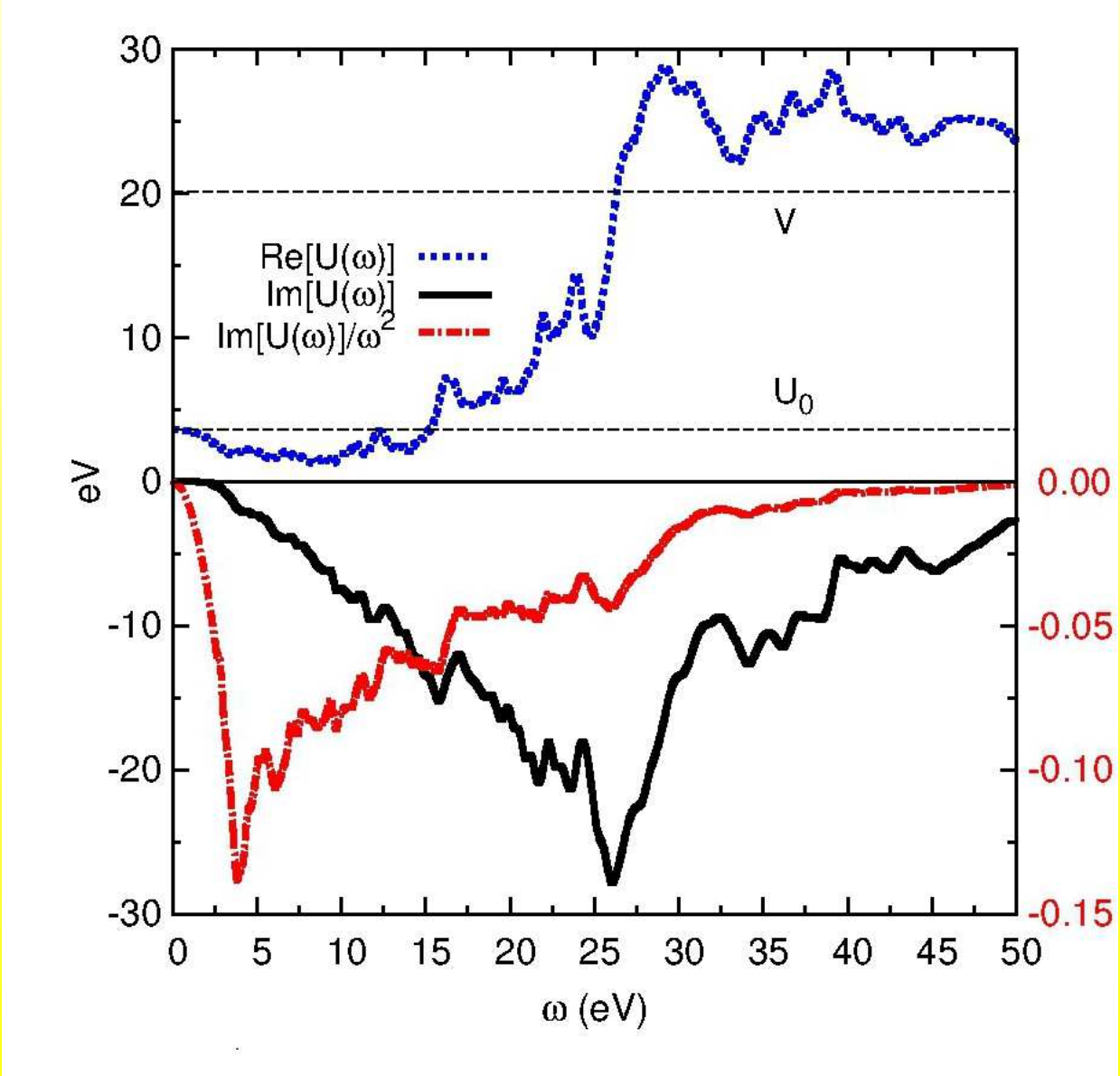
F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. B., A.I. Lichtenstein, PRB 2004

L. Vaugier, H. Jiang, SB, in preparation

BaFe2As2

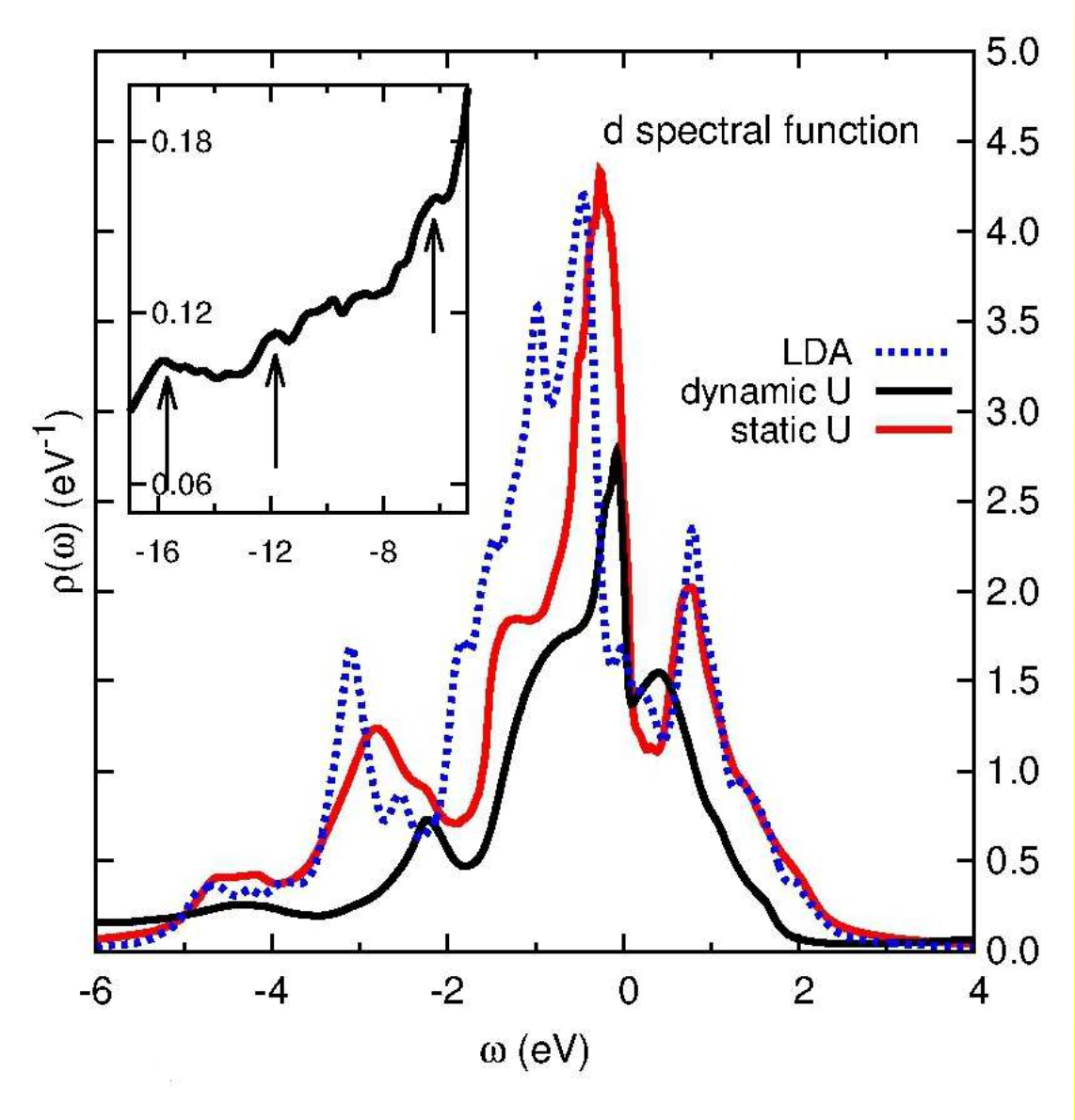


BaFe2As2: dynamical interaction



Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

K-doped BaFe2As2: spectral function



Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

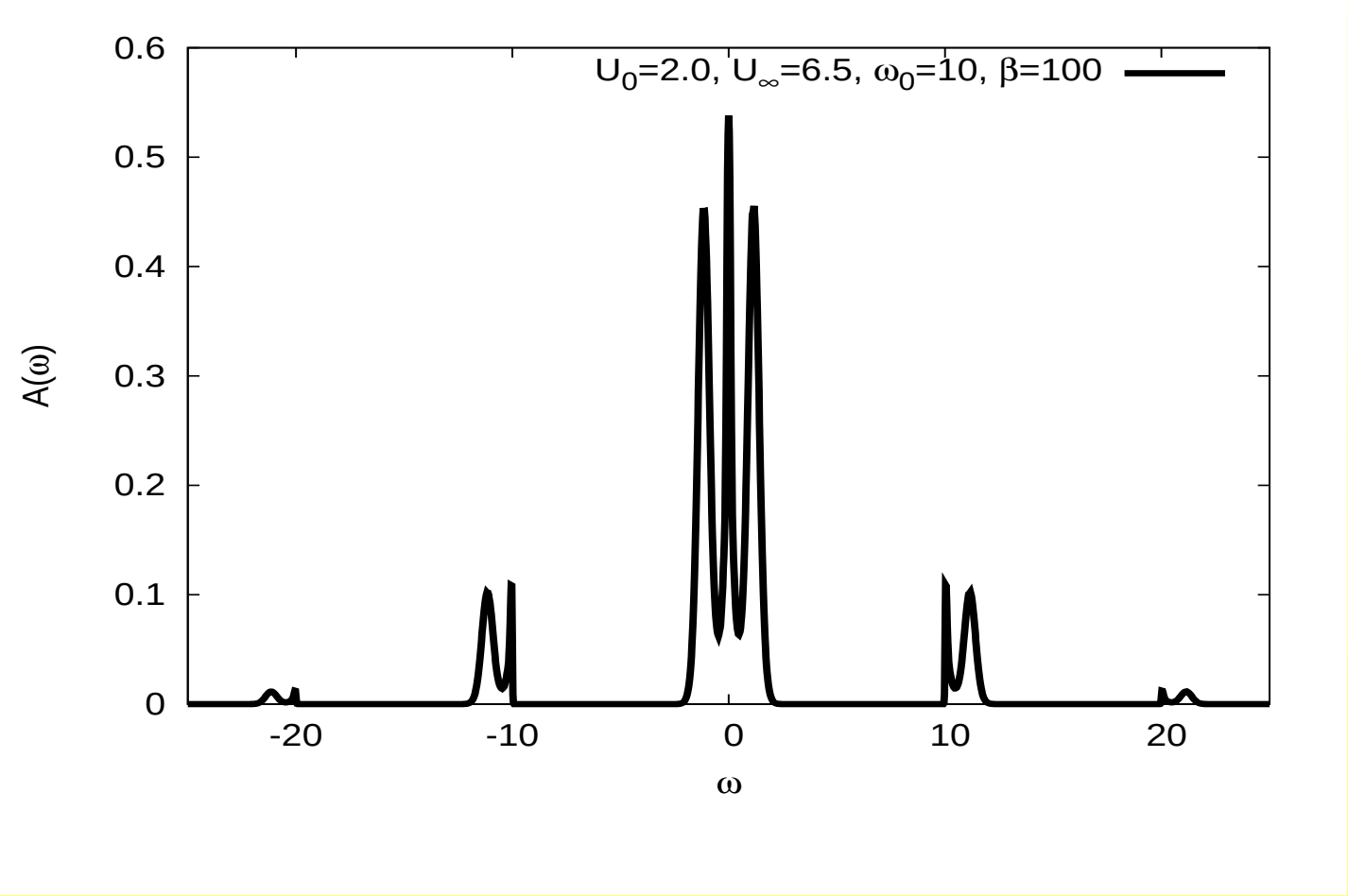
Hamiltonian formulation

$$
\begin{aligned}
H &= \sum_{\{im\sigma\}} (H^{\text{LDA}}_{im,i'm'} - H^{\text{double counting}}_{im,i'm'}) a^\dagger_{im\sigma} a_{i'm'\sigma} \\
&+ \frac{1}{2} \sum_{\substack{imm'\sigma \\ \text{(correl. orb.)}}} V^i_{mm'} n_{im\sigma} n_{im'-\sigma} \\
&+ \frac{1}{2} \sum_{\substack{im\neq m'\sigma \\ \text{(correl. orb.)}}} (V^i_{mm'} - J^i_{mm'}) n_{im\sigma} n_{im'\sigma} \\
&+ \sum_i \int d\omega \left[\lambda_{i\omega} (b^\dagger_{i\omega} + b_{i\omega}) \sum_{m\sigma} n_{im\sigma} + \omega b^\dagger_{i\omega} b_{i\omega} \right].
\end{aligned}
$$

with $-\text{Im}U_{\text{retarded}}(\omega) = \pi\lambda^2_\omega$, and $U_0 = V - 2\int d\omega \frac{\lambda^2_\omega}{\omega}$.

Effects of dynamic U?

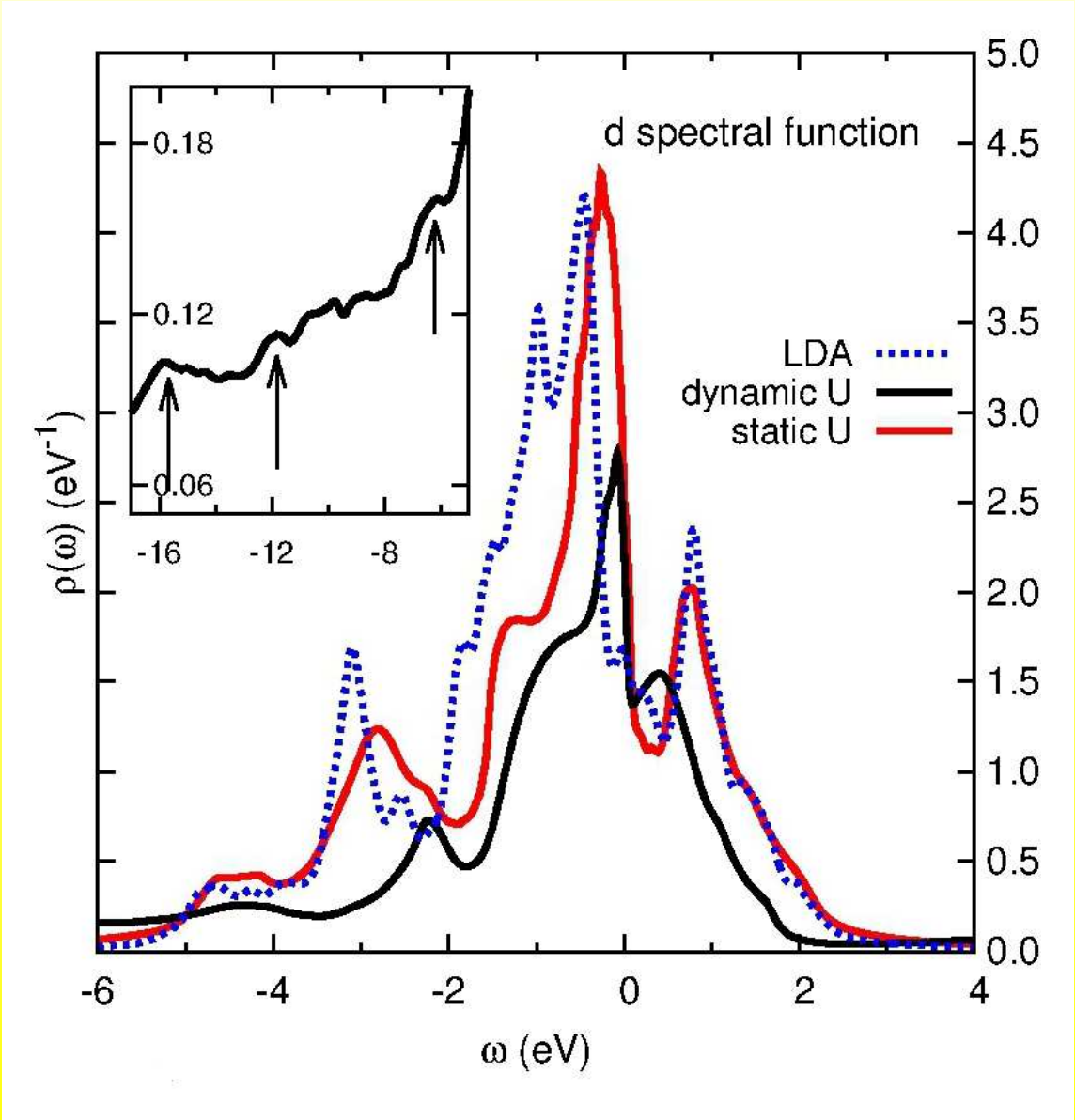
Hubbard-Holstein model in the “screening” (antiadiabatic) regime (large plasma frequency)



plasmon satellites at multiples of plasma frequency

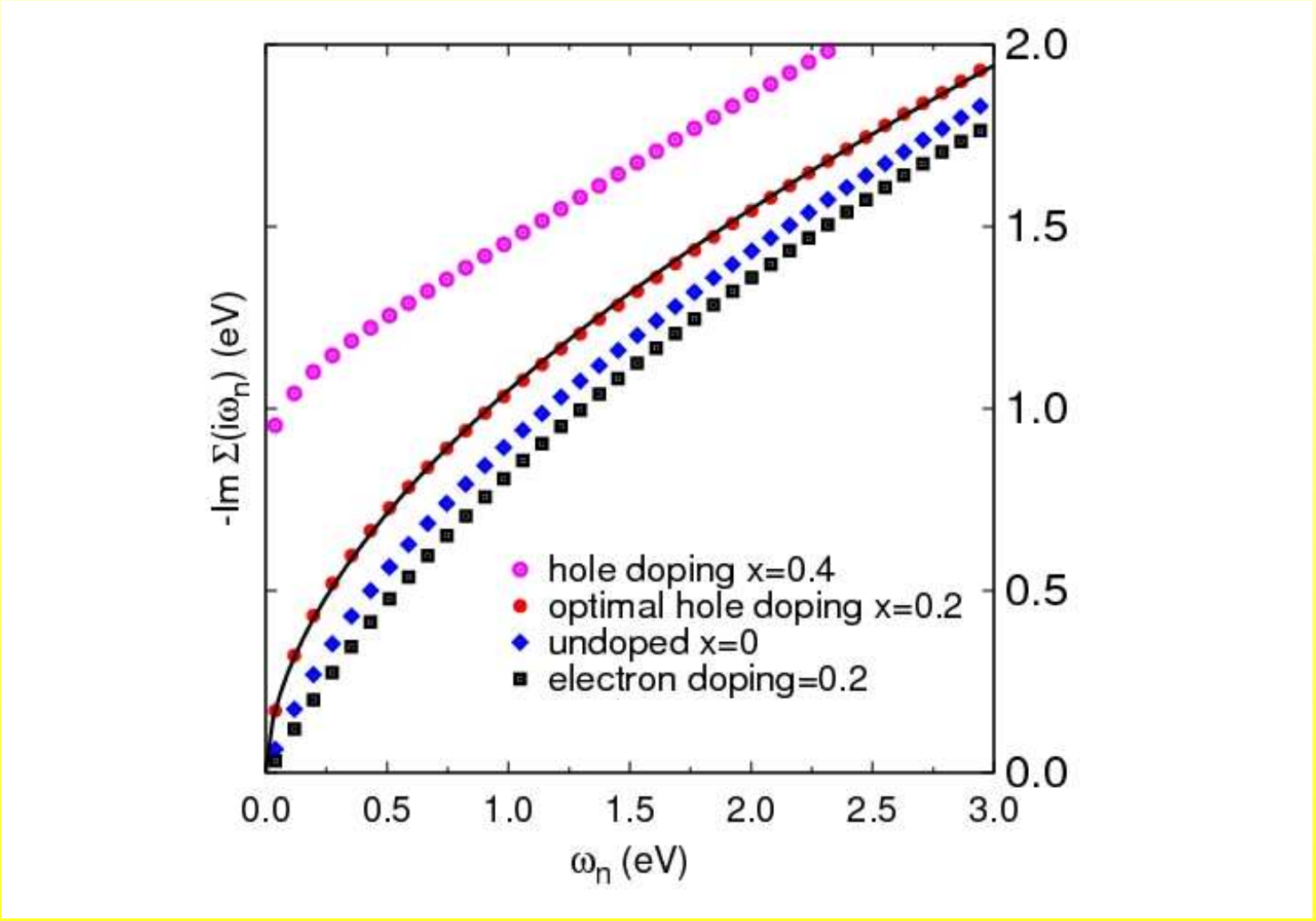
(M. Casula, A. Rubtsov, SB, PRB 2012)

K-doped BaFe2As2: spectral function



Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

K-doped BaFe2As2: self-energies

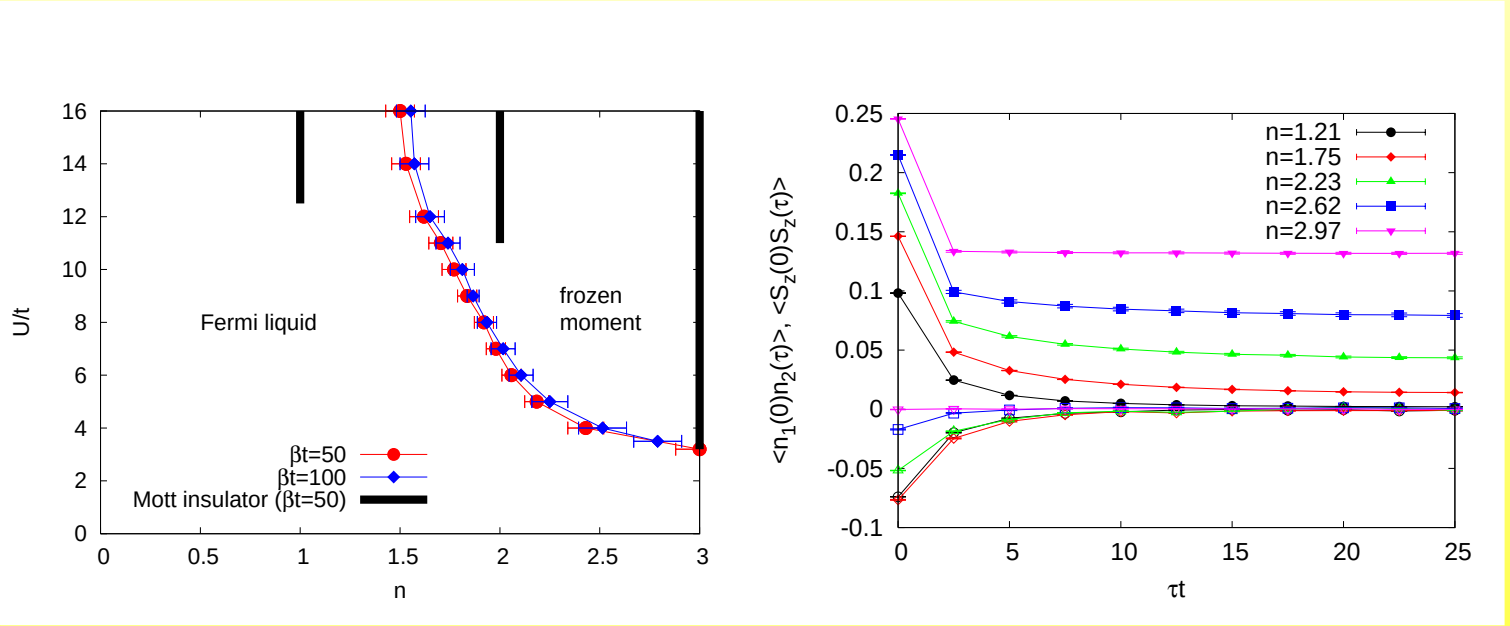


Optimally doped $Ba_{1-x}K_xFe2As2$: at the onset of square-root self-energy behavior!

Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

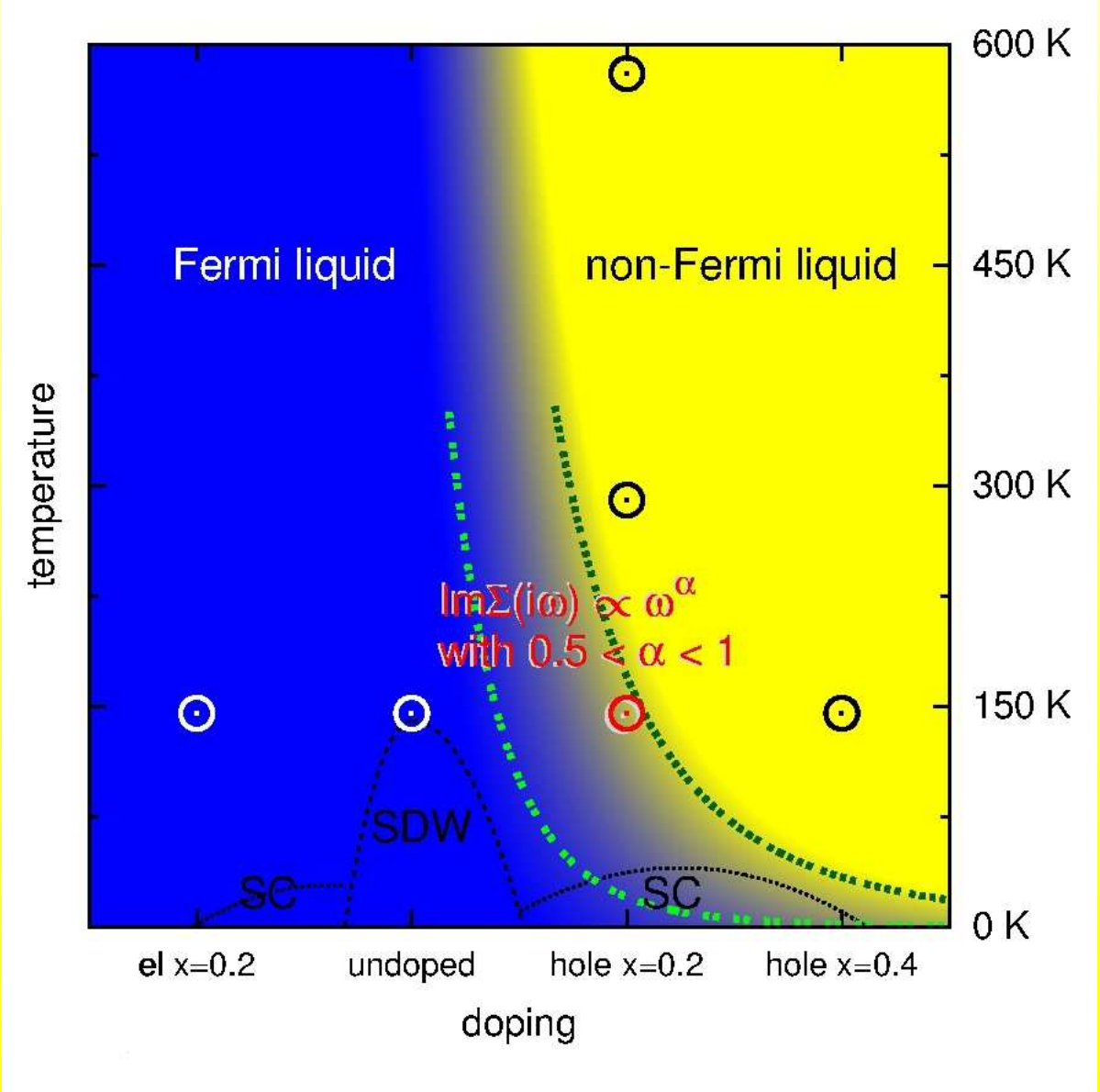
“Spin-freezing scenario”

seen in 3-band model (Werner and Millis, 2008): non-Fermi liquid phase with local moments



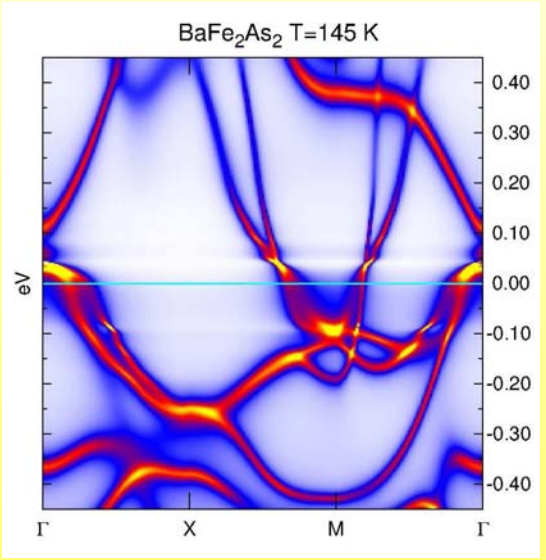
(cf cours)

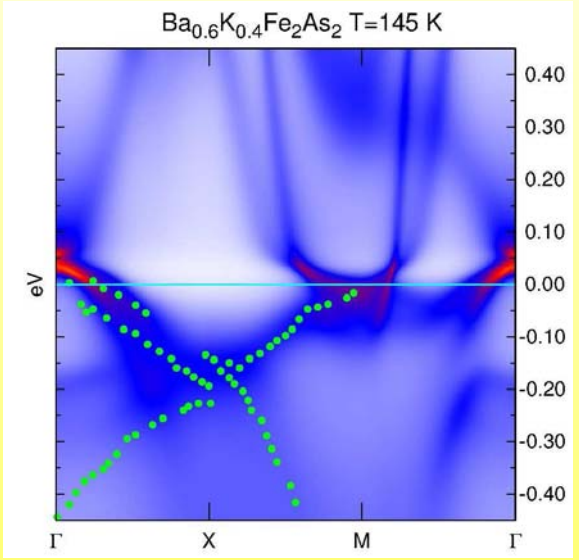
BaFe2As2: doping and T-dependence

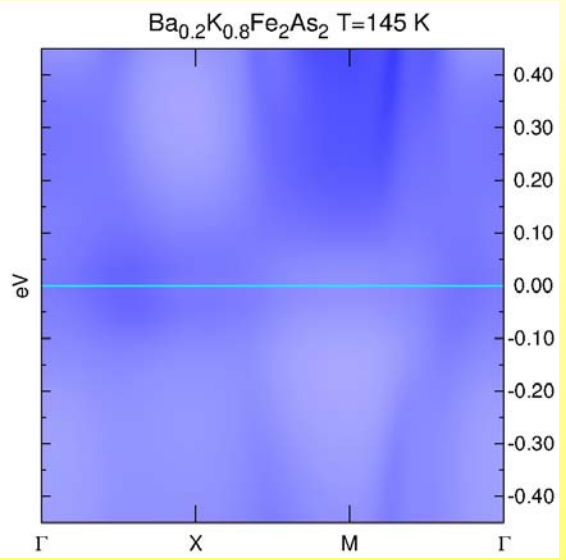


Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

K-doped BaFe2As2: k-resolved spectra



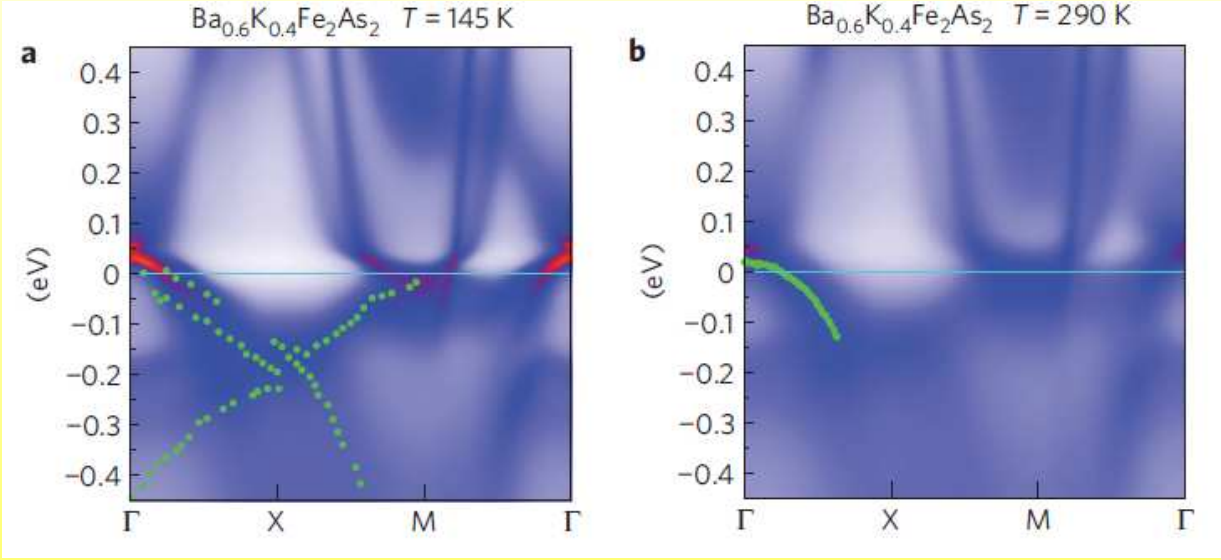




x = 0 x = 0.4 x = 0.8

Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

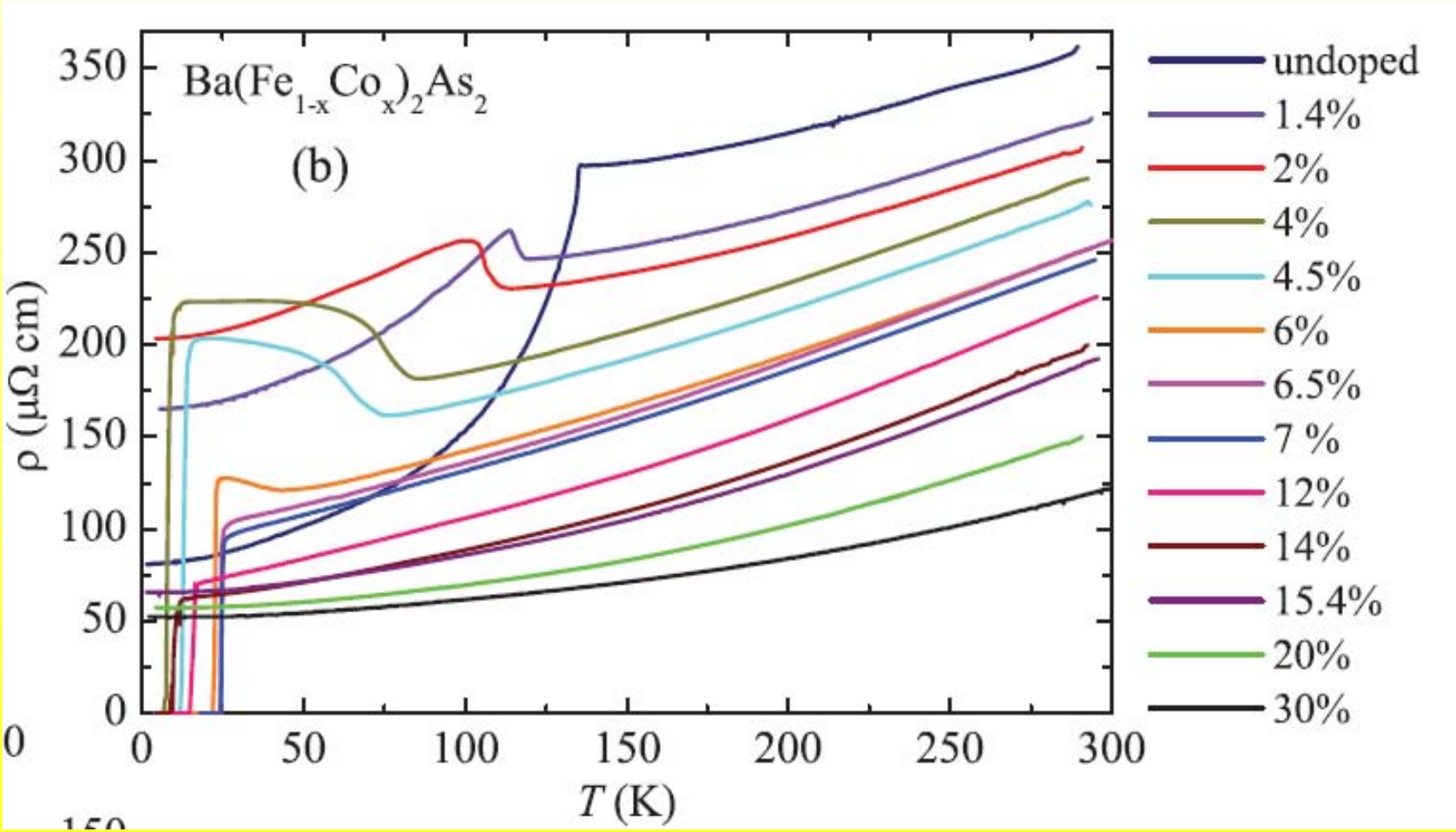
K-doped BaFe2As2: k-resolved spectra



Werner, Casula, Miyake,

Aryasetiawan, Millis, SB, Nature Phys. 2012

Resistivities?



A. Olariu, F. Rullier-Albenque, D. Colson, A. Forget, PRB 2011

Resistivities?

PHYSICAL REVIEW B **84**, 184512 (2011)

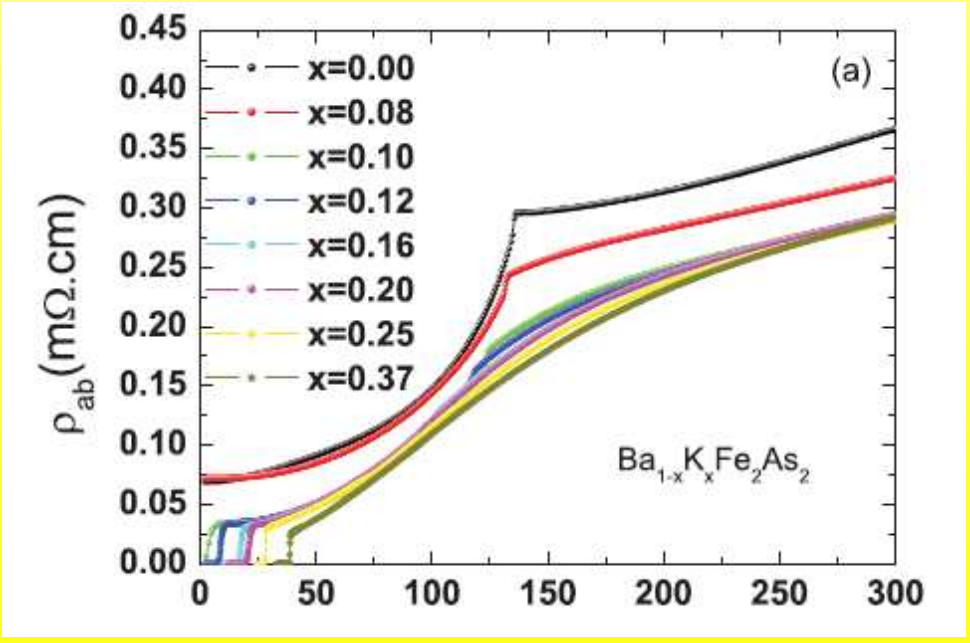
Transport properties and asymmetric scattering in $Ba_{1-x}K_xFe_2As_2$ singl

Bing Shen,[1] Huan Yang,[2] Zhao-Sheng Wang,[1] Fei Han,[1] Bin Zeng,[1] Lei Shan,[1] Cong Ren,[1] and

[1]*Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academ*

P.O. Box 603, Beijing 100190, China

[2]*National Laboratory for Solid State Microstructures, Department of Physics, Nanjing University, 21009*



Resistivities?

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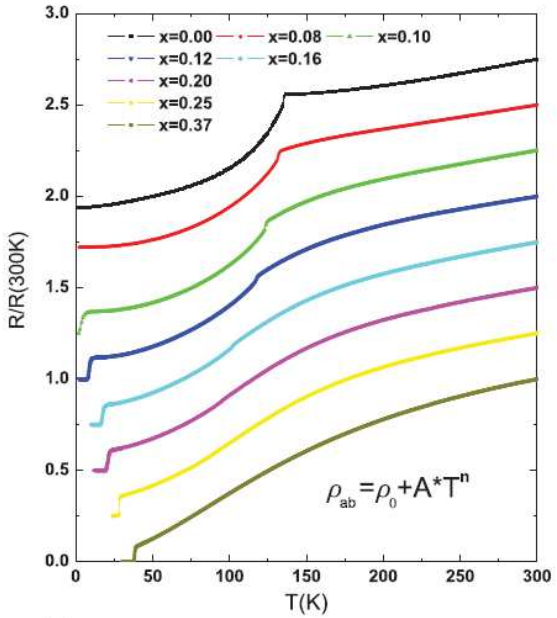
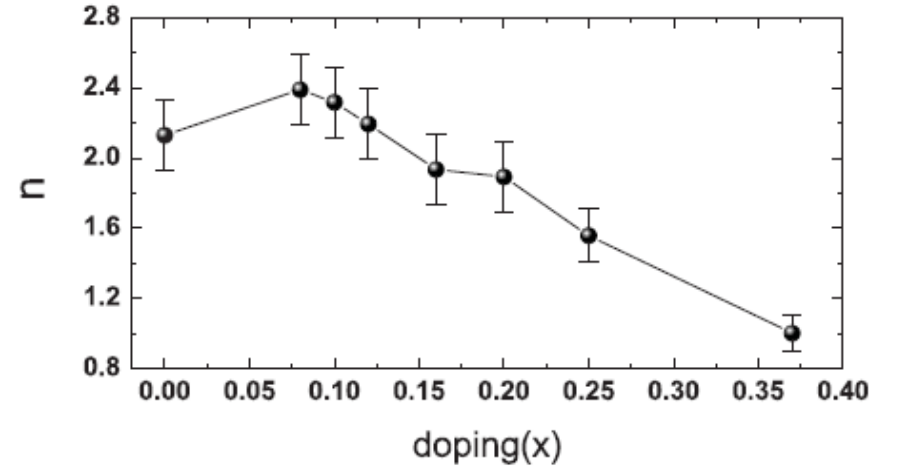
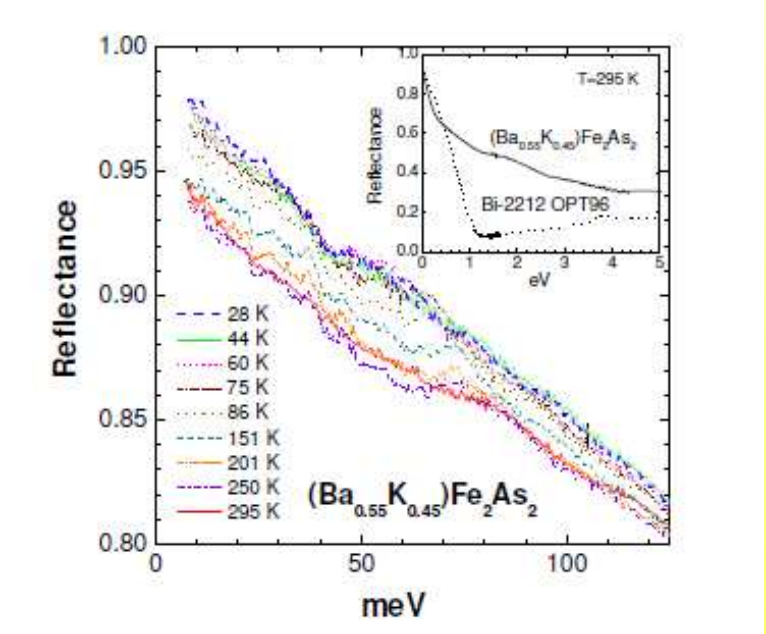
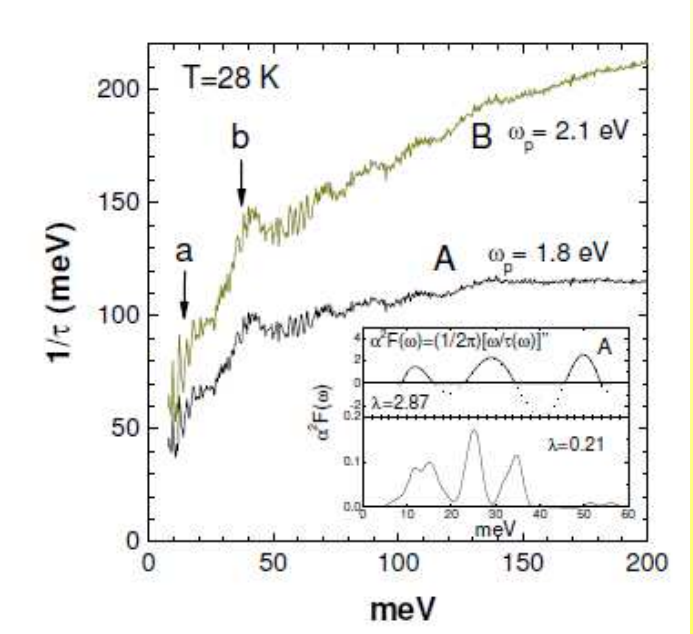


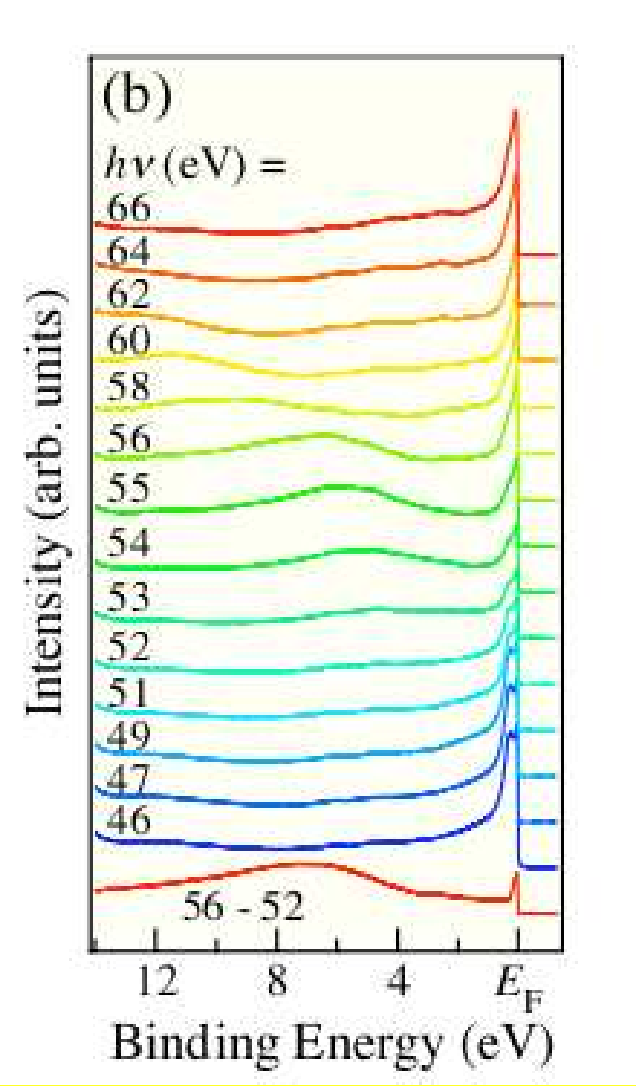


Optics?


Reflectance
meV
28 K
44 K
60 K
75 K
86 K
151 K
201 K
250 K
295 K
(Ba0.55K0.45)Fe2As2
T=295 K
Bi-2212 OPT96
eV

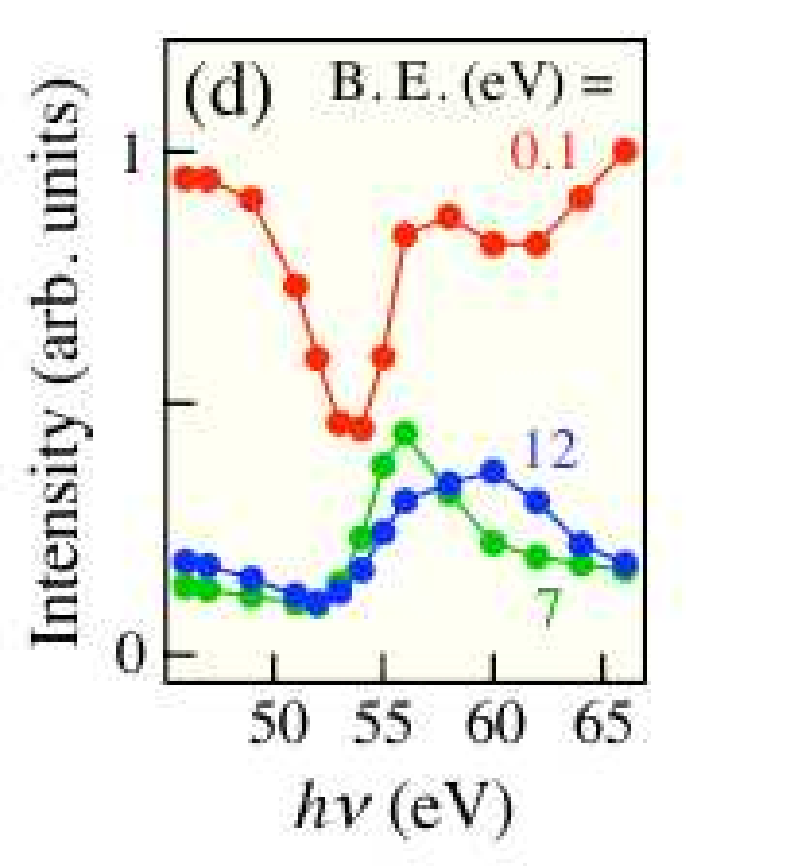

T=28 K
a
b
B ωp= 2.1 eV
A ωp= 1.8 eV
1/τ (meV)
meV
λ=2.87
λ=0.21
A

Satellites in BaFe2As2 ?



H. Ding's group

Satellites in BaFe2As2 ?



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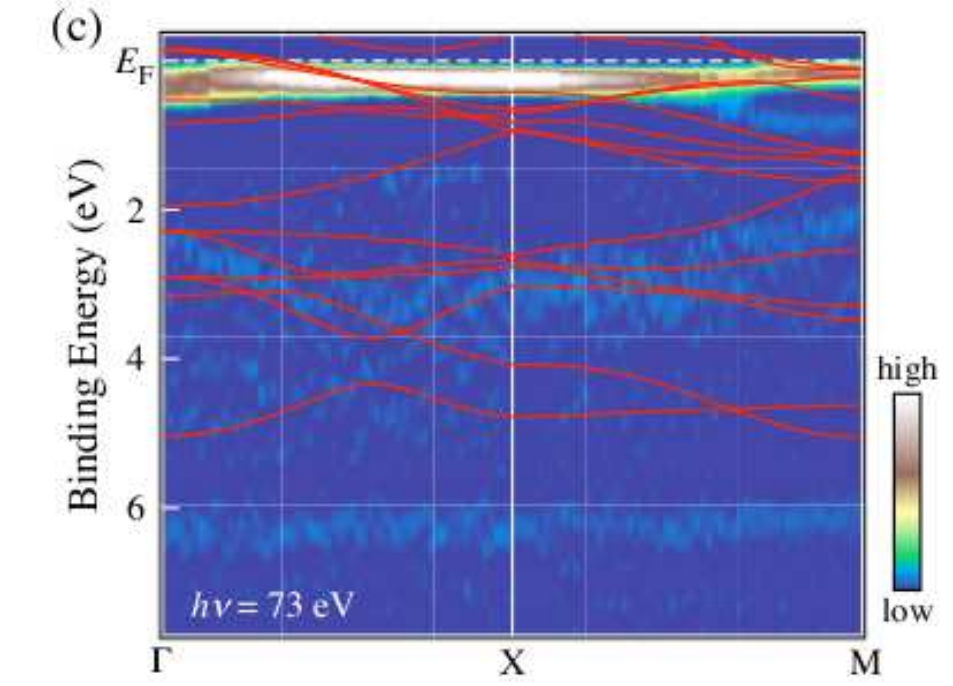
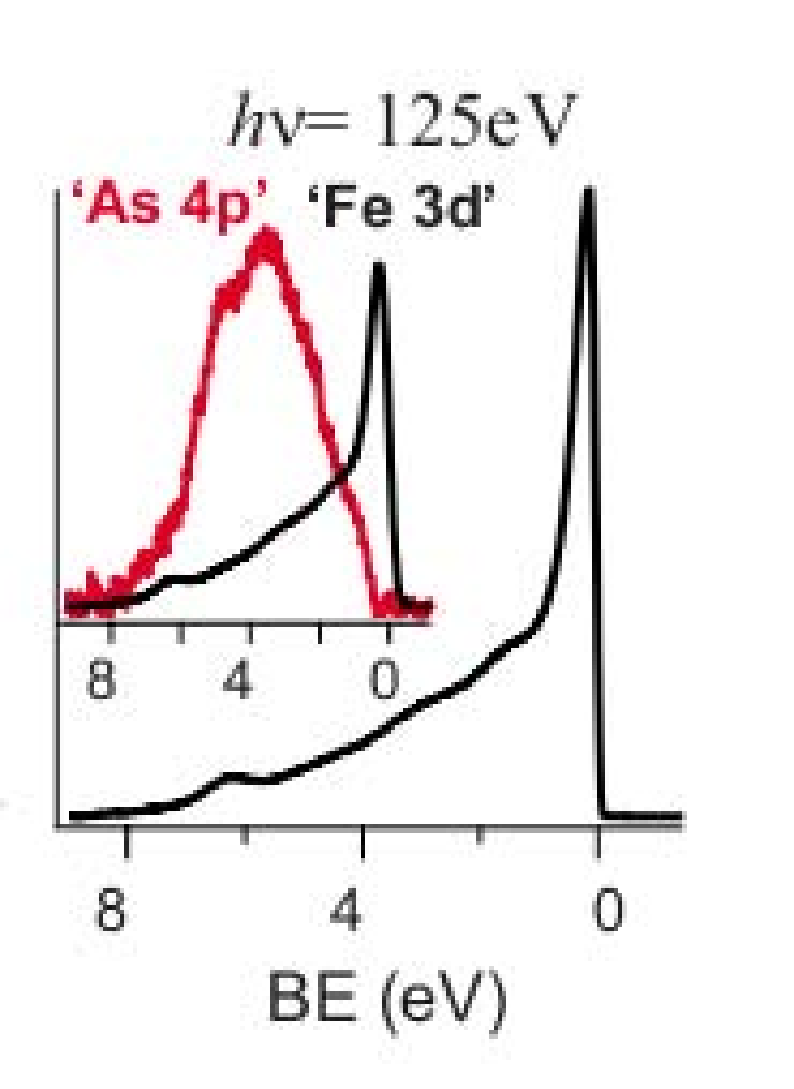


H. Ding's group

Satellites in BaFe2As2 ?



de Jong et al., PRB 2009

Effective Hamiltonian ?

Question:

Can we obtain the low-energy physics from an effective model with *static* U ?

- Which U ?
- Which one-particle Hamiltonian ?

M. Casula, P. Werner, L. Vaugier, F. Aryasetiawan, A. Millis, SB, arXiv 2012.

Hubbard-Holstein Hamiltonian

$$H = -\sum_{ij\sigma} t_{ij} d^\dagger_{i\sigma} d_{j\sigma} + V \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} + \mu \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma}$$
$$+ \omega_0 \sum_i b^\dagger_i b_i + \lambda \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} (b_i + b^\dagger_i). \qquad (2)$$

Lang-Firsov transformation:
$H \to H_{LF} = e^S H e^{-S}$ with
$S = -\frac{\lambda}{\omega_0} \sum_{i\sigma} n_{i\sigma} (b_i + b^\dagger_i)$

$$H_{\rm LF} = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U_0 \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} + \omega_0 \sum_i b^\dagger_i b_i, \tag{3}$$

with screened interaction $U_0 = V - \frac{2\lambda^2}{\omega_0}$.

and polaron operators

$c^\dagger_{i\sigma} = \exp(\frac{\lambda}{\omega_0}(b^\dagger_i - b_i))d^\dagger_{i\sigma}$

$c_{i\sigma} = \exp(\frac{\lambda}{\omega_0}(b_i - b^\dagger_i))d_{i\sigma}$.

Low-energy sector:

$$H_{\text{eff}} = \langle 0|H|0\rangle \quad (4)$$

$$= -\sum_{ij\sigma} Z_B t_{ij} d^\dagger_{i\sigma} d_{j\sigma} + U_0 \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} \quad (5)$$

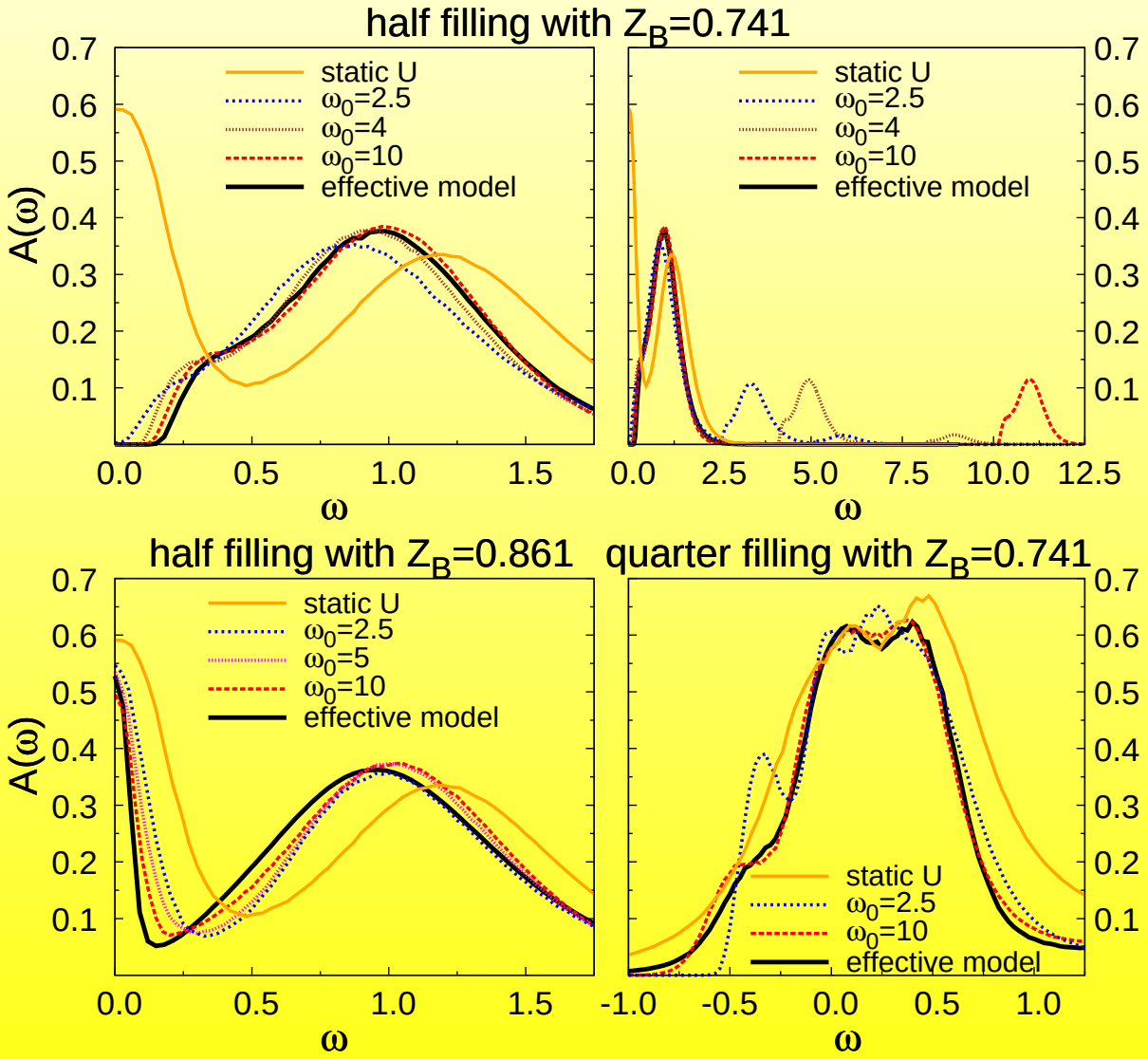
where $Z_B = \exp(-\lambda^2/\omega_0^2)$.

$$G_{ij}^{\text{low-energy}}(\tau) = -Z_B \langle T d_i(\tau) d_j^\dagger(0)\rangle_{H_{\text{eff}}}, = Z_B G_{ij}^{\text{eff}}(\tau) \quad (6)$$

Spectral function:

$$A^{\text{low-energy}}(\omega) = -\frac{1}{\pi}\text{Im}G^{\text{low-energy}} = -\frac{Z_B}{\pi}\text{Im}G^{\text{eff}} \quad (7)$$

Spectral functions



for various ω_0, $U_0 = 2$, Z_B as indicated.

Realistic Hamiltonian?

$$\left(p^\dagger d^\dagger\right) \begin{pmatrix} \mathcal{T}_{pp} & \mathcal{T}_{pd} \\ \mathcal{T}_{pd}^\dagger & \mathcal{T}_{dd} \end{pmatrix} \begin{pmatrix} p \\ d \end{pmatrix}, \tag{8}$$

Rescale!

$$(p^\dagger d^\dagger) \begin{pmatrix} \mathcal{T}_{pp} & \sqrt{Z_B}\mathcal{T}_{pd} \\ \sqrt{Z_B}\mathcal{T}_{pd}^\dagger & Z_B\mathcal{T}_{dd} \end{pmatrix} \begin{pmatrix} p \\ d \end{pmatrix}, \qquad (9)$$

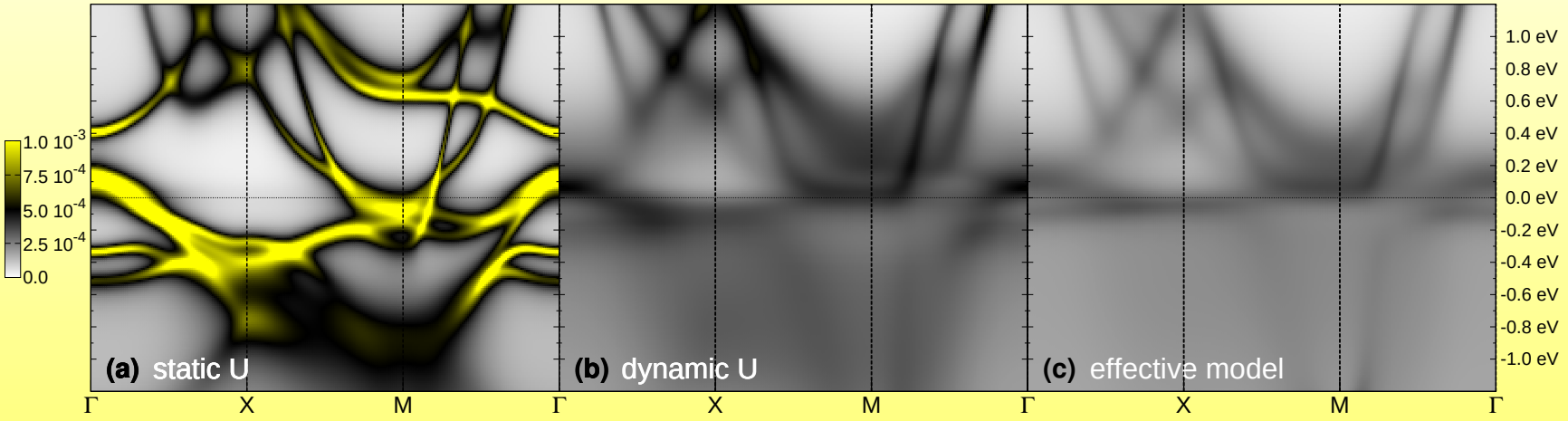
General dynamic U:

$$
\begin{aligned}
U_0 &= V + 2/\pi \int_0^\infty d\nu \, \mathrm{Im} U_{\mathrm{ret}}(\nu)/\nu, = U(\omega = 0) \\
Z_B &= \exp\left(1/\pi \int_0^\infty d\nu \, \mathrm{Im} U_{\mathrm{ret}}(\nu)/\nu^2 \right) .
\end{aligned}
$$

Materials??

	Z_B	ω_0	$V = U(\infty)$	$U_0 = U(0)$	$U_{\text{literature}}$
$SrVO_3$	0.70	18.0	16.5	3.3	4 - 5
Sr_2VO_4	0.70	18.1	15.7	3.1	4.2
$LaVO_3$	0.57	10.3	13.3	1.9	5
VO_2	0.67	15.6	15.2	2.7	4
TaS_2	0.79	14.7	8.4	1.5	
$SrMnO_3$	0.50	13.3	21.6	3.1	2.7
$BaFe_2As_2$	0.59	15.7	19.7	2.8	5
LaOFeAs	0.61	16.5	19.1	2.7	3.5 - 5
FeSe	0.63	17.4	20.7	4.2	4 - 5
CuO	0.63	21.1	26.1	6.8	7.5

BaFe2As2



spectral function for $K_{0.4}Ba_{0.6}Fe_2As_2$: static U standard DMFT calculation, DMFT calculation with dynamic $U(\omega)$, and effective low-energy model.

M. Casula, P. Werner, L. Vaugier, F. Aryasetiawan, A. Millis, SB, arXiv 2012.

Some previous calculations ...

... compensated for missing bandwidth renormalisation effect by choosing an artificially enhanced U

Dynamical U

- shifts spectral weight to higher energies
- explicit extended DMFT calculations possible
- effective static model: $U_{stat} = U(0)$, one-particle part renormalized by
  $Z_B = \exp\left(1/\pi \int_0^\infty d\nu \, \mathrm{Im}U_{\mathrm{ret}}(\nu)/\nu^2\right)$
  (single-mode case: $Z_B = \exp(-\lambda^2/\omega_0^2)$)
- solves puzzle about "too small" cRPA U-values!

M. Casula, A. Rubtsov, SB., PRB 2012.

P. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. Millis, SB, Nature Physics 2012.

M. Casula, P. Werner, L. Vaugier, F. Aryasetiawan, A. Millis, SB, arXiv 2012.

Conclusions

Towards a quantitative description of correlated materials from first principles:

- LaFeAsO: moderately correlated metal
- FeSe: Hubbard band!
- BaFe2As2: dynamical screening effects, doping-dependent (in)coherence

Methodology:

- From LDA+DMFT to LDA+$\mathcal{U}(\omega)$+DMFT
- Hubbard $\mathcal{U}(\omega)$ from constrained RPA

Collaborators and references

- LaFeAsO vs. LaFePO: trends and models in LDA

  Vildosola, Pourovskii, Arita, Biermann, Georges, PRB 2008

- LaFeAsO: assessing correlations in LDA+DMFT

  Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Georges, Miyake, SB, PRB 2009

- FeSe – strongly correlated?

  Aichhorn, SB, Miyake, Georges, Imada, PRB 2010.

- d- and f-electron correlations in REFeAsO

  Pourovskii, Vildosola, SB, Georges, EPL 2009. Miyake, Pourovskii, Vildosola, SB, Georges, JPSJ 2009.

- Ru-doping in $BaFe_2As_2$: reduction of correlations

  V. Brouet, F. Rullier-Albenque, M. Marsi, B. Mansart, M. Aichhorn, SB., J. Faure, L. Perfetti, A. Taleb-Ibrahimi, P. Le Fevre, A. Forget, D. Colson, PRL 2010

References

- Dynamical screening in correlated materials:
  M. Casula, A. Rubtsov, SB, PRB 2012.
- $BaFe_2As_2$
  P. Werner, M. Casula, T. Miyake, F. Aryasetiawan, A. Millis, SB, Nat. Phys. 2012.
- Constrained random phase approximation ...:
  F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. B., A.I. Lichtenstein, PRB 2004
- ... and its implementation into Wien2k:
  L. Vaugier, H. Jiang, SB, to be published
- Effective model:
  M. Casula, P. Werner, L. Vaugier, F. Aryasetiawan, A. Millis, SB, arXiv 2012.