ES&ES 2013

V. V. Nemoshkalenko Memorial Conference and Workshop
Electronic Structure and Electron Spectroscopies

May 20-23, 2013, Institute of Metal Physics, Kyiv, Ukraine

Electronic structure and superconductivity of iron based superconductors: pnictides versus chalcogenides and similar new systems

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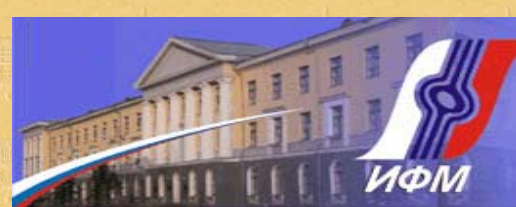
Collaborators: E.Z. Kuchinskii, I.A. Nekrasov, N.S. Pavlov

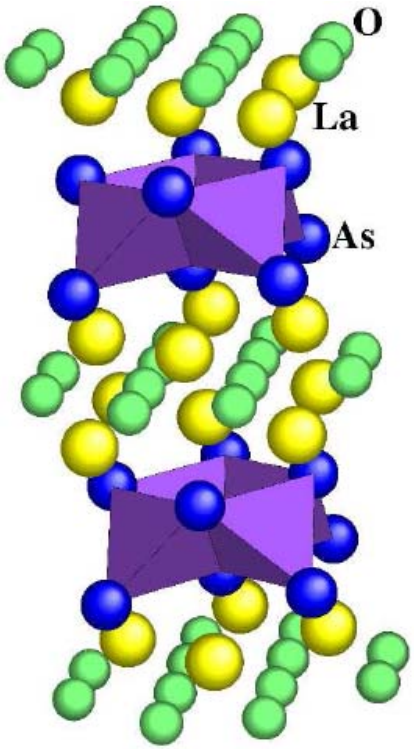
RUSSIAN ACADEMY OF SCIENCES
URALS DIVISION
Institute of Electrophysics



Outline of the talk

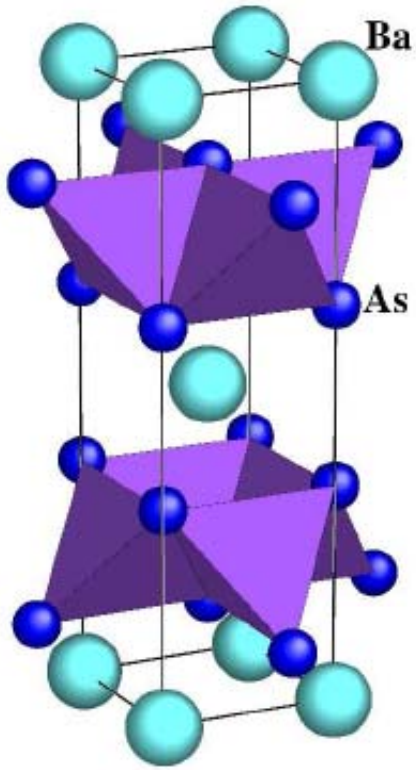
- Electronic structure of Fe-pnictides
  - Fermi surfaces and superconducting gaps
- Fe-chalcogenides: AFe_2Se_2 a new class?
  - Fermi surfaces
  - Antiferromagnetism and vacancies
  - Multiple phases
- Single layer FeSe!
- DOS – T_c correlation?
  - Multiple bands superconductivity
- New Pt,Pd-pnictides
- Conclusions

Essentially physics of FeAs layers!



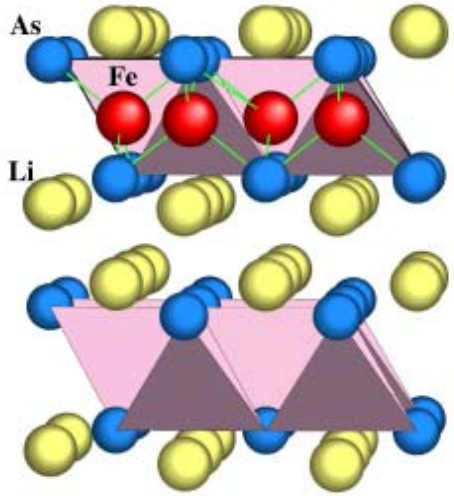
LaOFeAs

$(\mathrm{RE})^{+3}\mathrm{O}^{-2}\mathrm{Fe}^{+2}\mathrm{As}^{-3}$



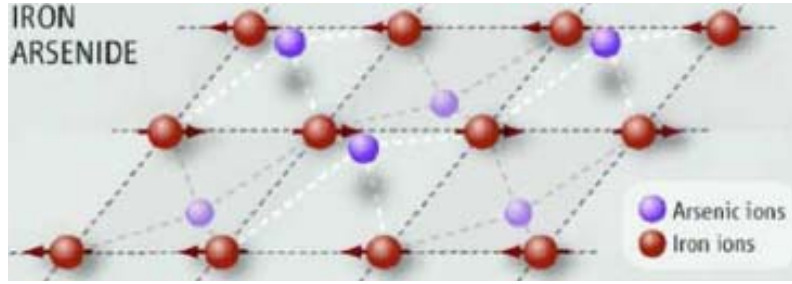
$BaFe_2As_2$

$Ba^{+2}(Fe^{+2})_2(As^{-3})_2$



LiFeAs

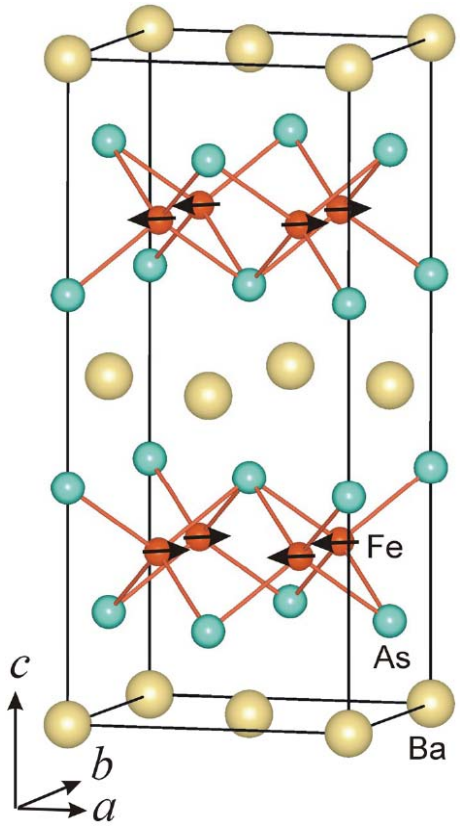
$Li^{+1}Fe^{+2}As^{-3}$



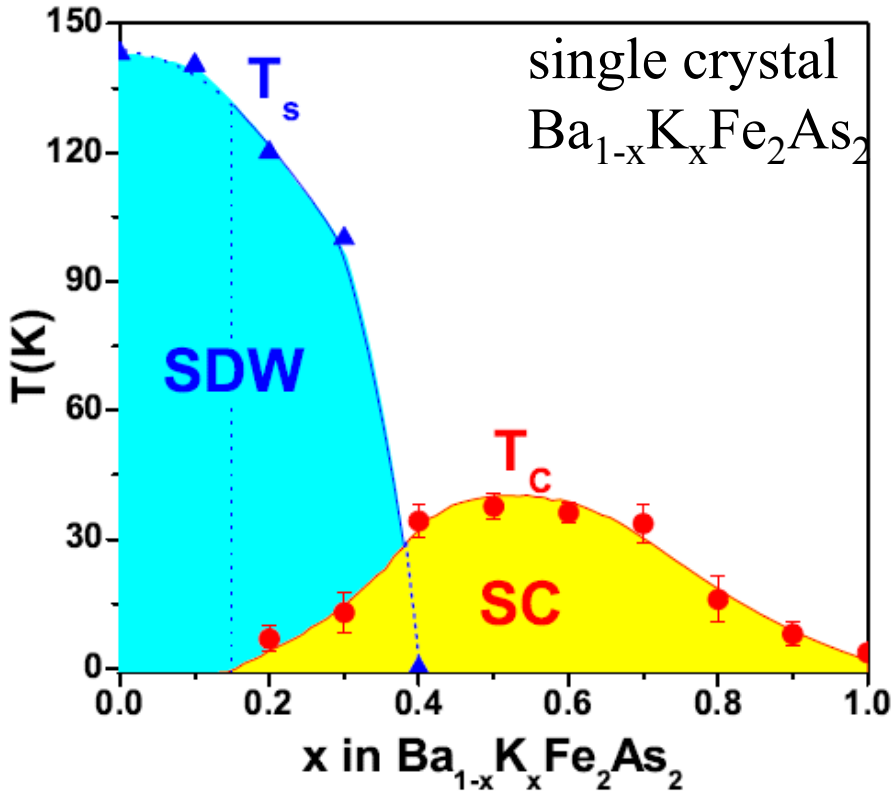
FeAs tetrahedra form two-dimensional layers surrounded by LaO, Ba or Li.
Fe ions inside tetrahedra form a square lattice.

Magnetic properties of 122

Neutron scattering



Q. Huang et al., arXiv:0806.2776 (2008)

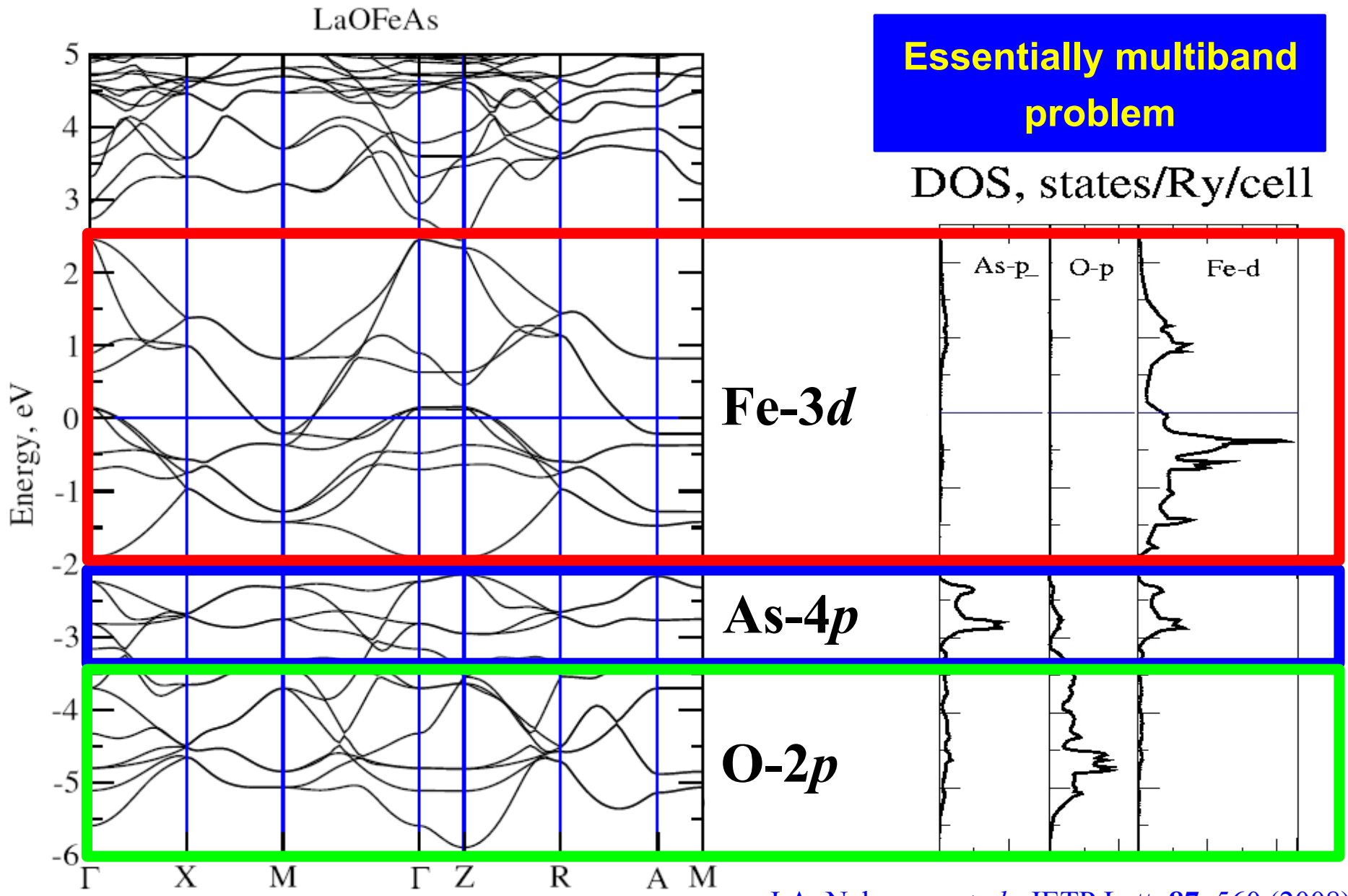


H. Chen et al., arXiv:0807.3950 (2008)

- 142K [220K][1] – T(*I4/mmm*)→O(*Fmmm*)
- 142K [220K][1] – AFM order of Fe with $\sqrt{2}a\times\sqrt{2}b\times 2c$ cell, stripes along b [a][1]
- m_{Fe}=0.87 μ_B at 5K for $BaFe_2As_2$
- m_{Fe}=0.94 μ_B at 10K for $SrFe_2As_2$

[1] for $SrFe_2As_2$, J. Zhao et al., PRB **78**, 140504 (2008)

LDA band structure of tetragonal LaOFeAs

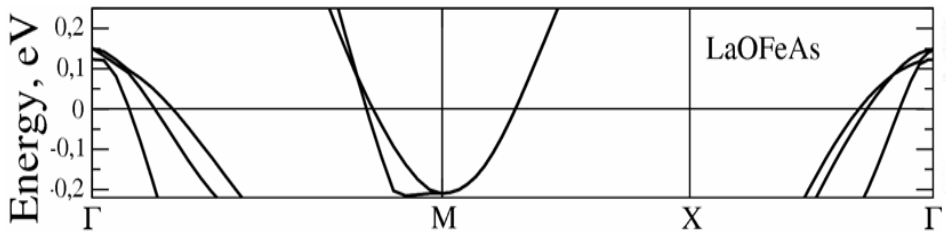


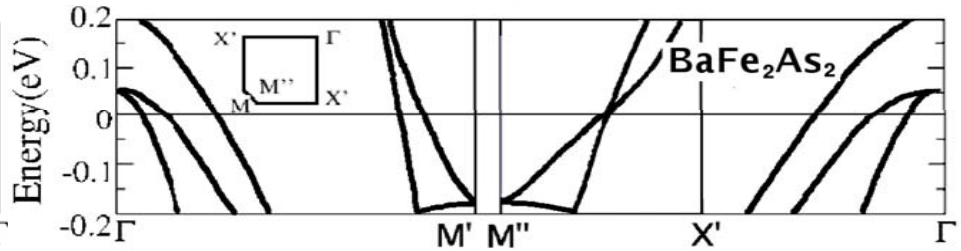
Essentially multiband problem

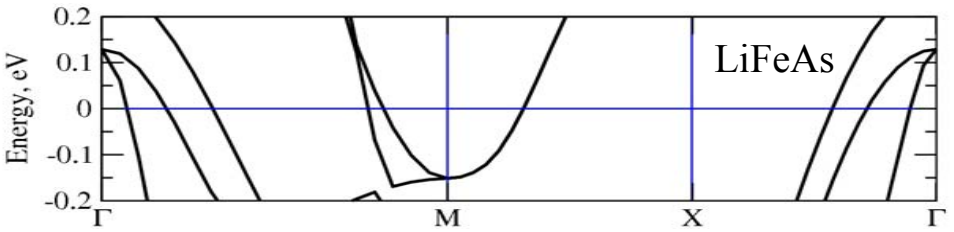
I.A. Nekrasov *et al.*, JETP Lett. **87**, 560 (2008)

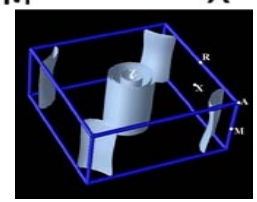
FeAs systems:

ReOFeAs	La	Ce	Pr	Nd
T_c, K	26	41	52	51.9

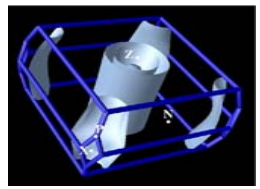




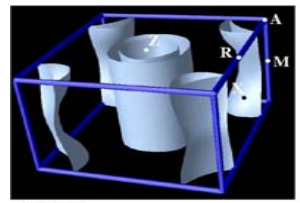




LaOFeAs



$BaFe_2As_2$



LiFeAs

Pnictogen height?

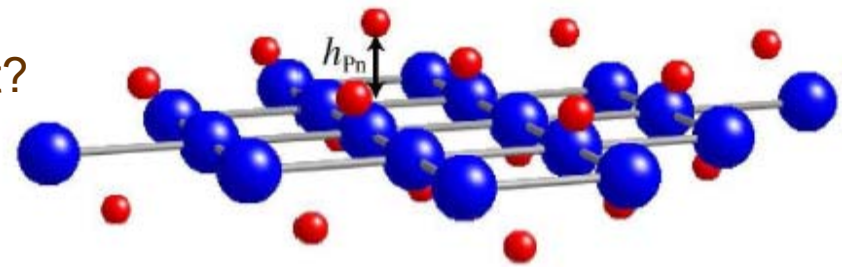
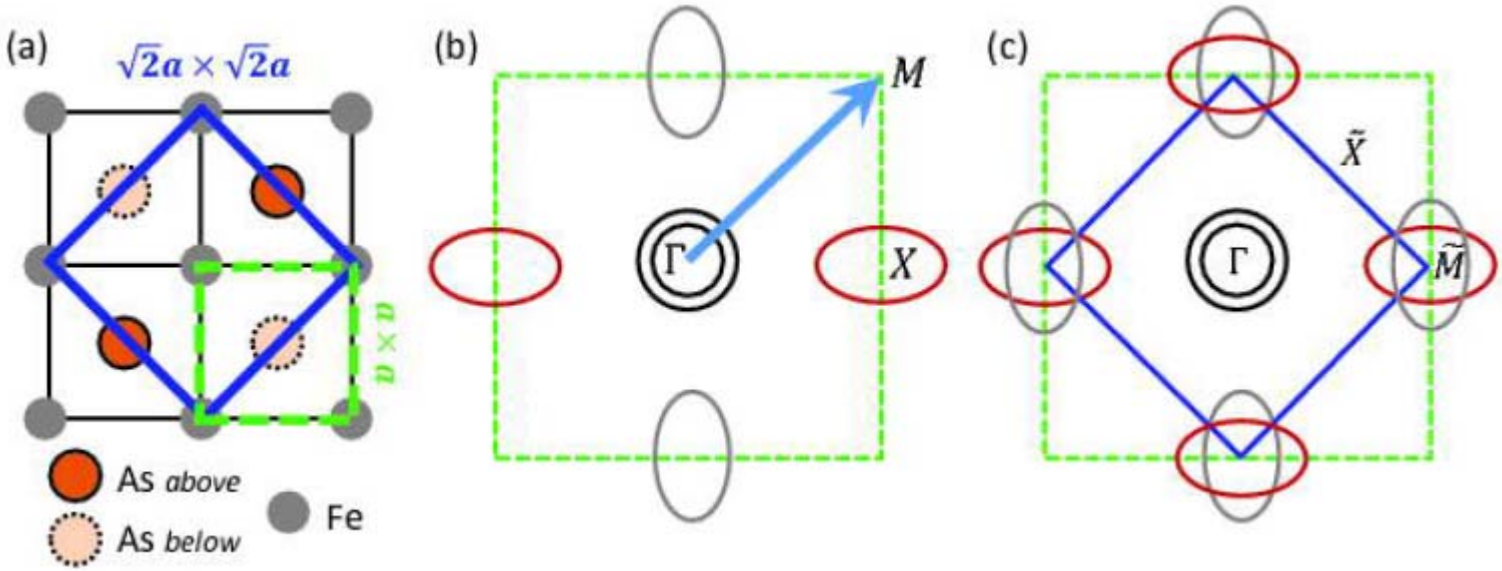


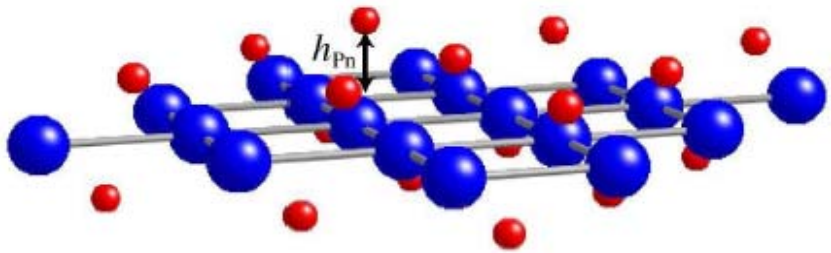
Fig. 5. LDA Brillouin zo



The simplest model accounting for distinct electron and hole Fermi surfaces would be a model in the 1-Fe zone with parabolic dispersions

$$H = \sum_{k,\sigma,i=\alpha_1,\alpha_2,\beta_1,\beta_2} \varepsilon_k^i c_{ik\sigma}^\dagger c_{ik\sigma}.$$

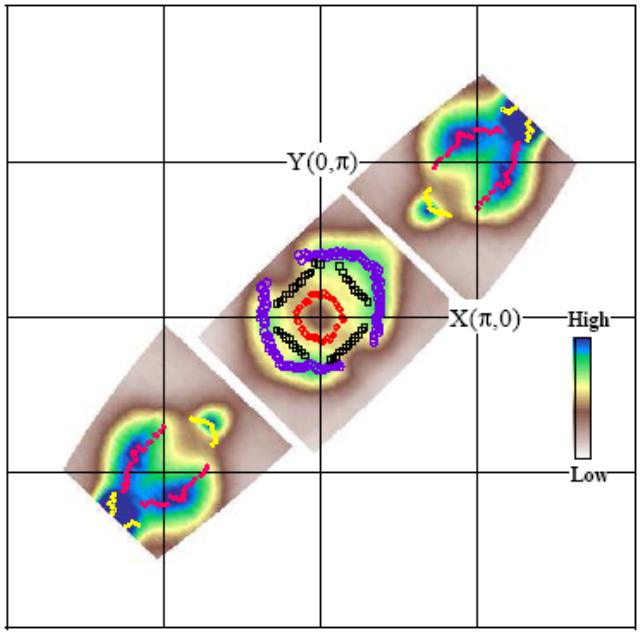
Here, $c_{ik\sigma}$ is the annihilation operator for an electron with momentum $\boldsymbol{k}$, spin σ, and band index i, $\varepsilon_k^{\alpha_{1,2}} = -\frac{k^2}{2m_{1,2}} + \mu$, $\varepsilon_k^{\beta_1} = \frac{(k_x-\pi/a)^2}{2m_x} + \frac{k_y^2}{2m_y} - \mu$, and $\varepsilon_k^{\beta_2} = \frac{k_x^2}{2m_y} + \frac{(k_y-\pi/a)^2}{2m_x} - \mu$ are the dispersions of hole α_i and electron β_i bands.



Fermi Surface and Band Renormalization in (Sr,K)Fe_2As_2 Superconductor from Angle-Resolved Photoemission Spectroscopy

Haiyun Liu[1], Wentao Zhang[1], Lin Zhao[1], Xiaowen Jia[1], Jianqiao Meng[1], Guodong Liu[1], Xiaoli Dong[1], G. F. Chen[2], J. L. Luo[2], N. L. Wang[2], Wei Lu[1], Guiling Wang[3], Yong Zhou[3], Yong Zhu[4], Xiaoyang Wang[4], Zhongxian Zhao[1], Zuyan Xu[3], Chuangtian Chen[4], X. J. Zhou[1,*]

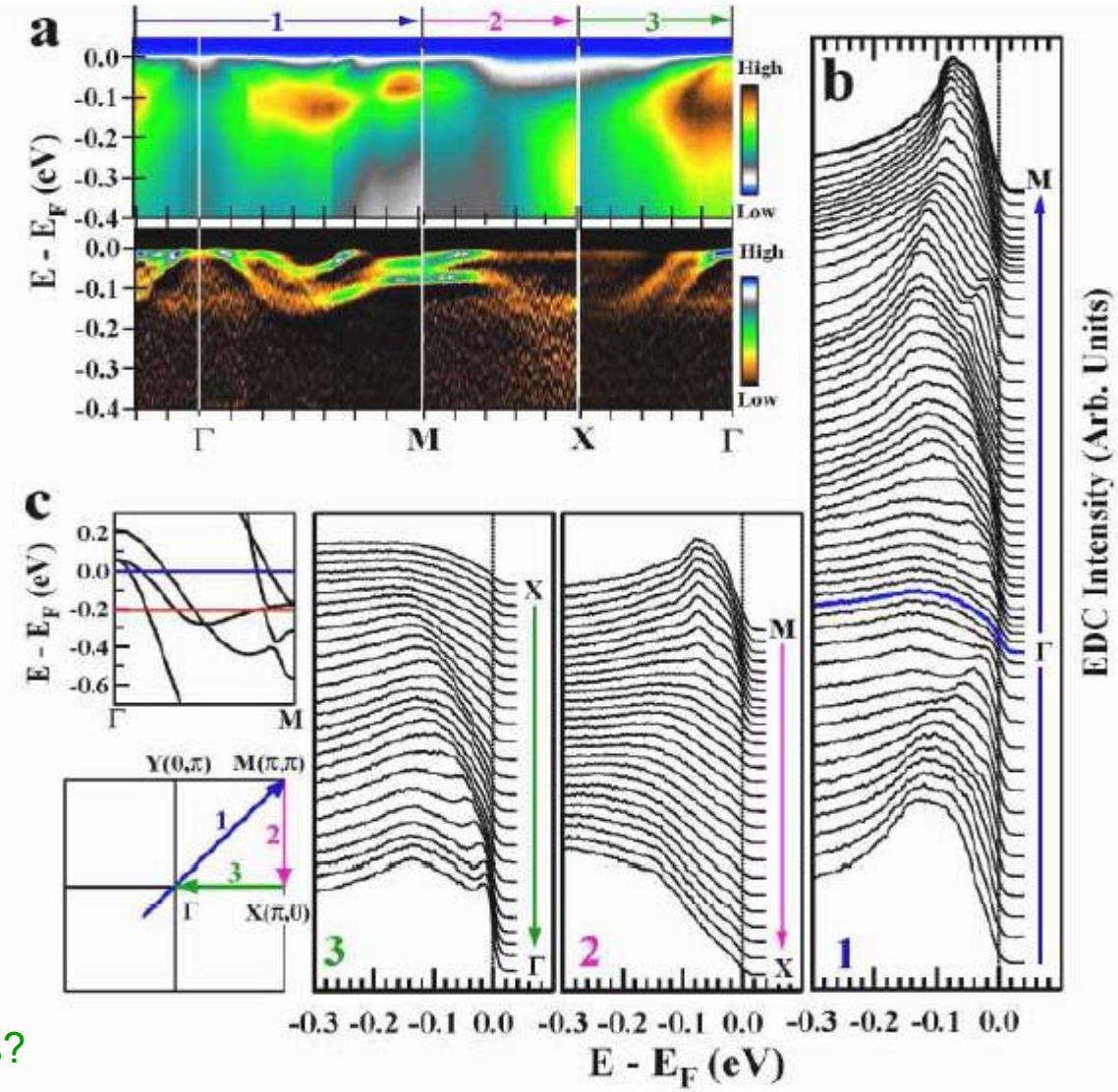
arXiv: 0806.4806



Three hole cylinders!

T_c=21 K

Band narrowing due to correlations?

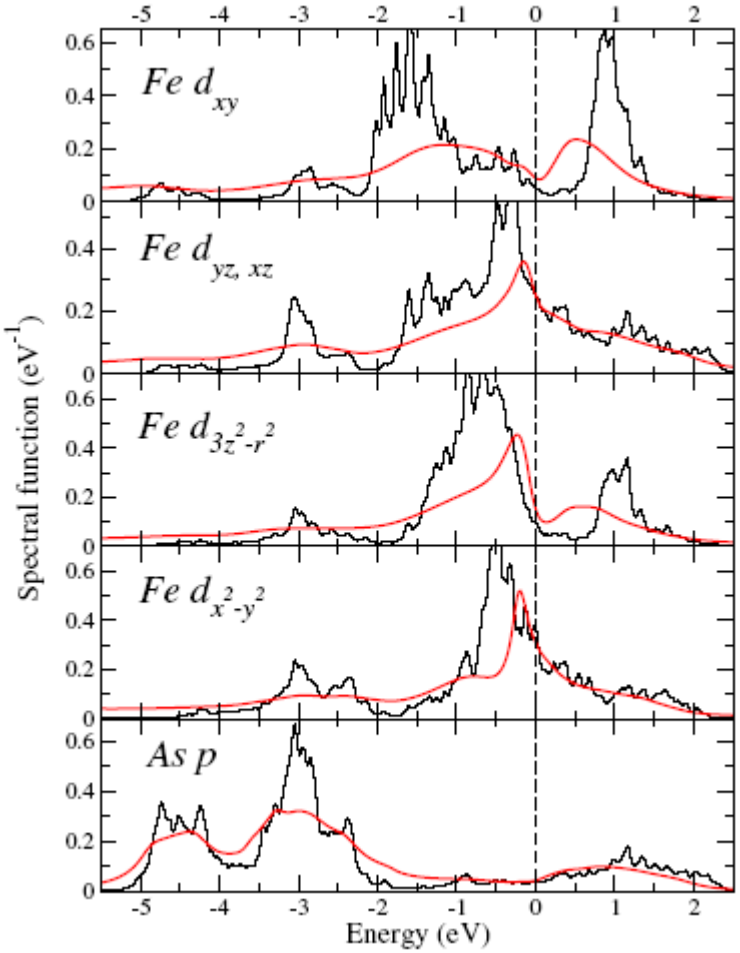


LDA+DMFT: strong or intermediate correlations?

PHYSICAL REVIEW B **80**, 092501 (2009)

Classification of the electronic correlation strength in the iron pnictides: The case of the parent compound $BaFe_2As_2$

S. L. Skornyakov,[1] A. V. Efremov,[1] N. A. Skorikov,[1] M. A. Korotin,[1] Yu. A. Izyumov,[1] V. I. Anisimov,[1] A. V. Kozhevnikov,[2] and D. Vollhardt[3]



$U=3.1$ eV and $J=0.81$ eV

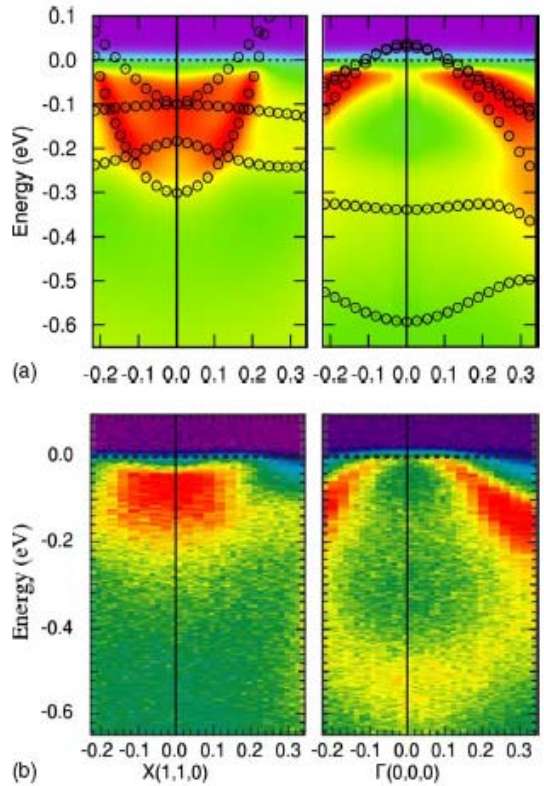


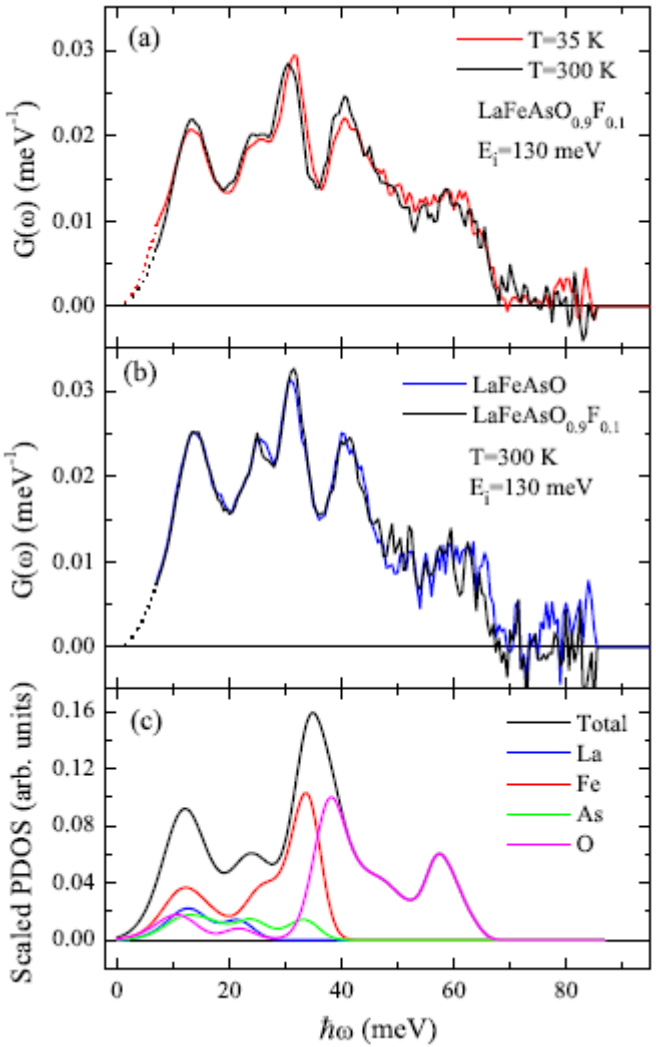
FIG. 3. (Color online) The **k**-resolved total spectral function $A(\mathbf{k},\omega)$ of $BaFe_2As_2$ near the Γ and X points in the Brillouin zone is depicted as a contour plot. Upper panel: LDA+DMFT spectral function including the renormalized band structure (circles) obtained by plotting the peak positions of the spectral function $A(\mathbf{k},\omega)$. Lower panel: The corresponding experimental ARPES intensity map of Liu *et al.* (Ref. 29).

Phonons

arXiv: 0807.3370

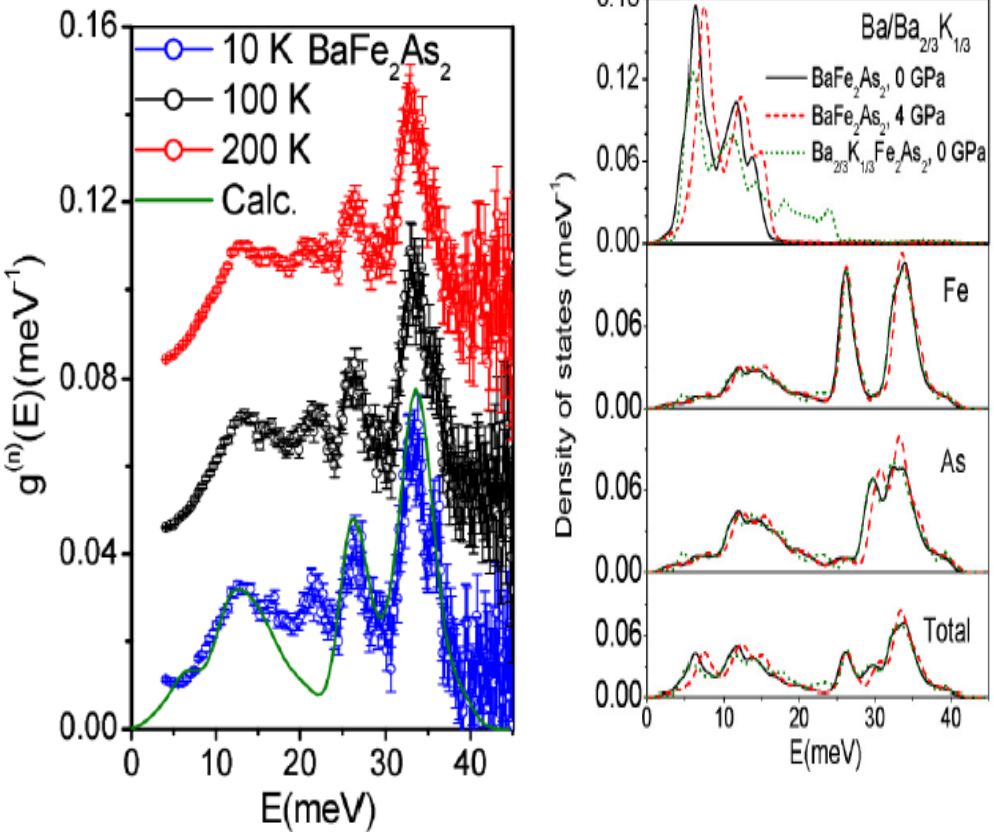
Phonon Density of States of $LaFeAsO_{1-x}F_x$

A. D. Christianson,[1] M. D. Lumsden,[1] O. Delaire,[2] M. B. Stone,[1] D. L. Abernathy,[1] M. A. McGuire,[1] A. S. Sefat,[1] R. Jin,[1] B. C. Sales,[1] D. Mandrus,[1] E. D. Mun,[3] P. C. Canfield,[3] J. Y. Y. Lin,[2] M. Lucas,[2] M. Kresch,[2] J. B. Keith,[2] B. Fultz,[2] E. A. Goremychkin,[4,5] and R. J. McQueeney[3]



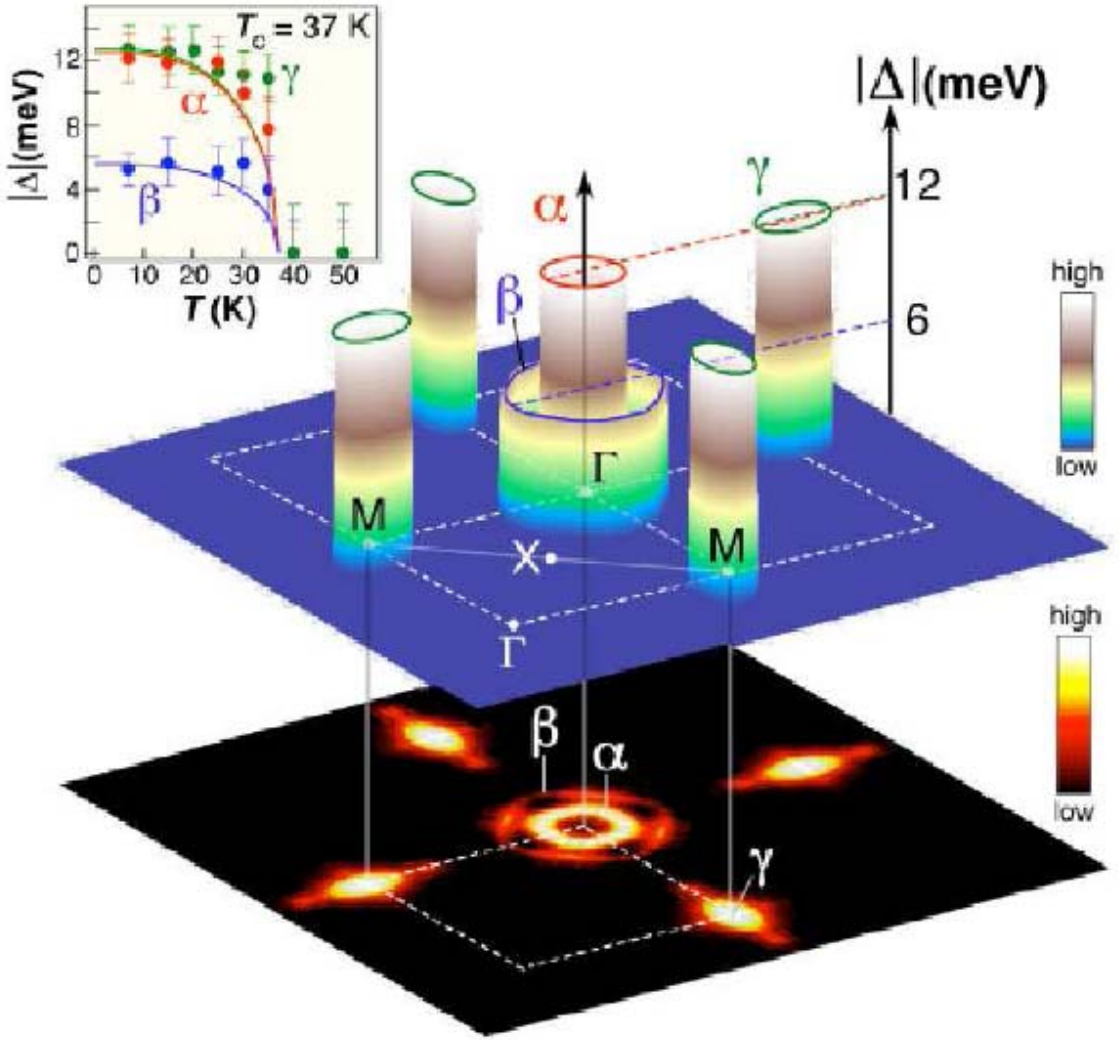
Inelastic neutron scattering and lattice dynamical calculations in $BaFe_2As_2$

R. Mittal[1], Y. Su[1], S. Rols[2], T. Chatterji[3], S. L. Chaplot[4], H. Schober[2], M. Rotter[5], D. Johrendt[5] and Th. Brueckel[1,6]



arXiv: 0807.3172

Superconducting gap – ARPES data



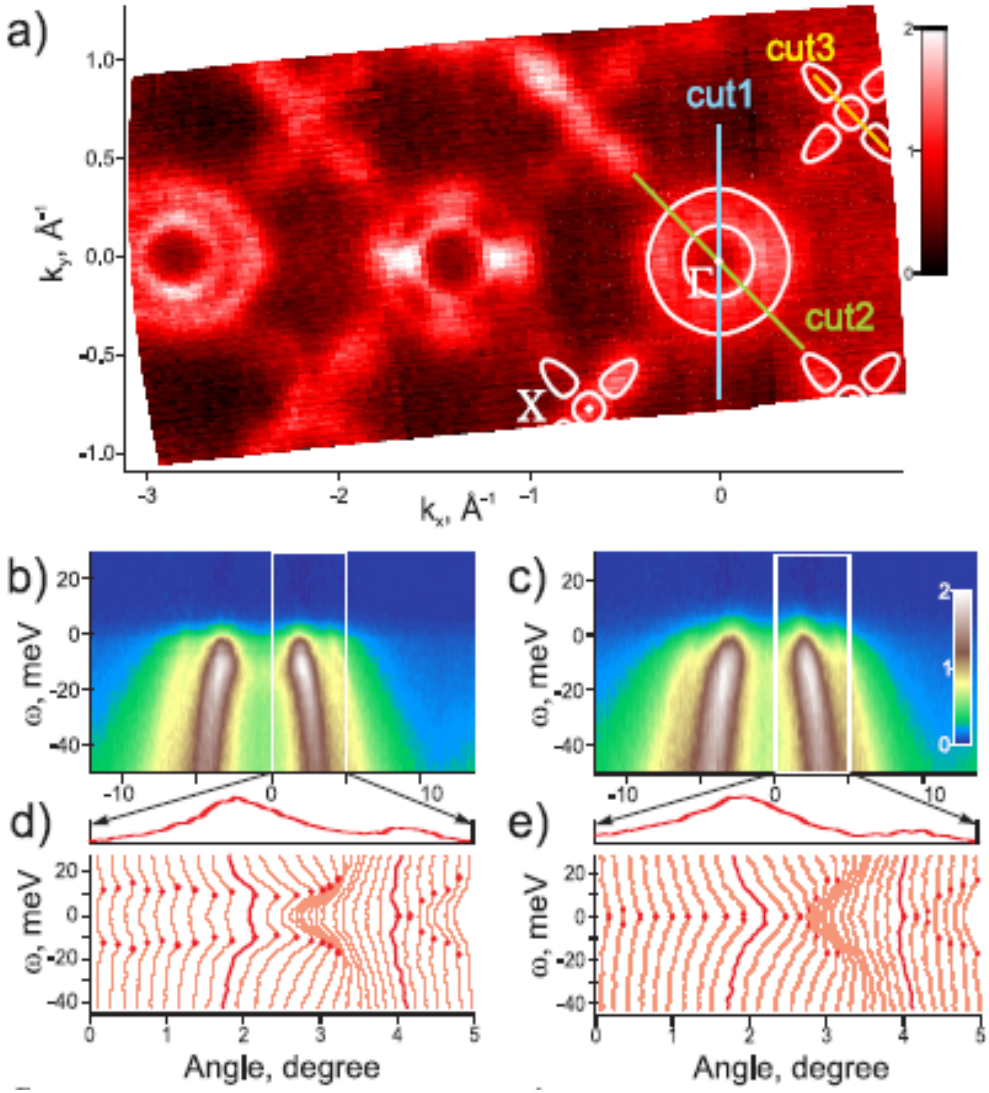
arXiv: 0807.0419

Schematic picture of superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$. Lower picture represents Fermi surfaces (ARPES intensity), upper insert – temperature dependence of gaps at different sheets of the Fermi surface.

arXiv: 0809.4455

Momentum dependence of the superconducting gap in $Ba_{1-x}K_xFe_2As_2$

D. V. Evtushinsky,[1] D. S. Inosov,[1,2] V. B. Zabolotnyy,[1] A. Koitzsch,[1] M. Knupfer,[1] B. Büchner,[1] G. L. Sun,[2] V. Hinkov,[2] A. V. Boris,[2] C. T. Lin,[2] B. Keimer,[2] A. Varykhalov,[3] A. A. Kordyuk,[1,4] and S. V. Borisenko[1]



Ref. num.	2	3	4	5	6	This paper
T_c	53 K	37 K	35 K	53 K	37 K	32 K
Inner Γ-barrel	20	12.5	12	15	12	9.2 ± 1
Outer Γ-barrel	—	5.5	8	—	6	<4
X-pocket	—	12.5	10	—	11	9 ± 2
Blades	—	—	(11)	—	—	~9
Gap anisotropy	—	<3	2	<5	<3	<1.5

Table I: Momentum dependence of the superconducting gap in iron-arsenic superconductors, as revealed by ARPES studies from five independent groups, sorted by the time of appearance on the arXiv.org. Values of the gap and estimates of the gap anisotropy on the inner Γ-barrel are given in millielectron-volts.

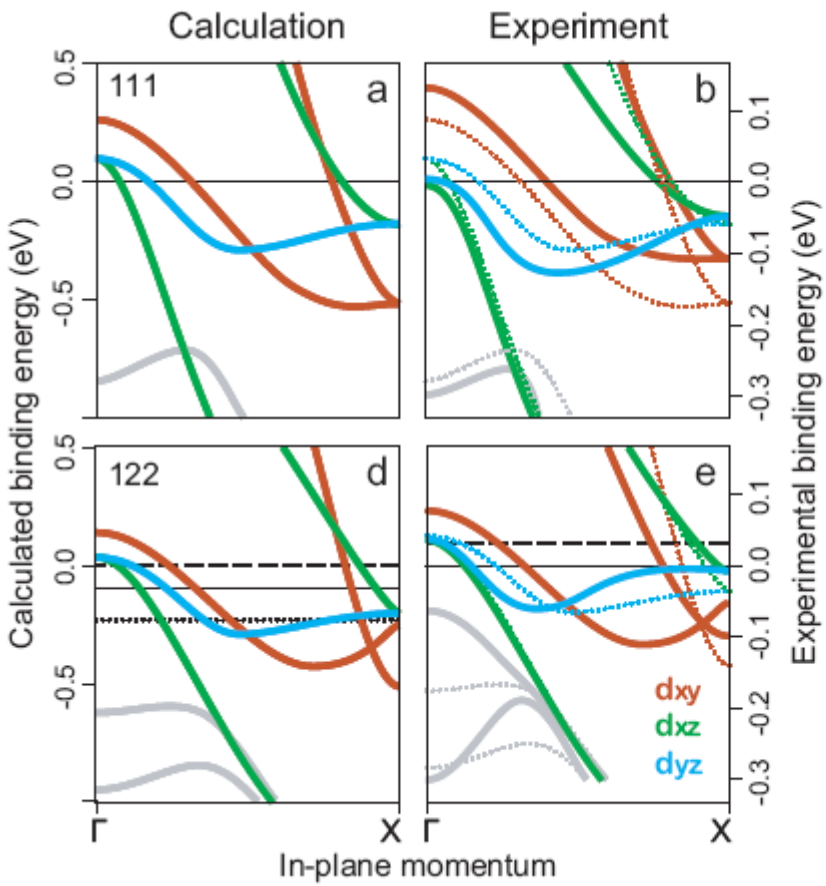
Ref. num.	2	3	4	5	6	7	8	9	This paper
Large gap	9	8.1	8.2	6.8	7.5	3.7	9.6	4	6.8
Small gap	—	3.6	5.5	—	3.9	—	3.4	—	<3

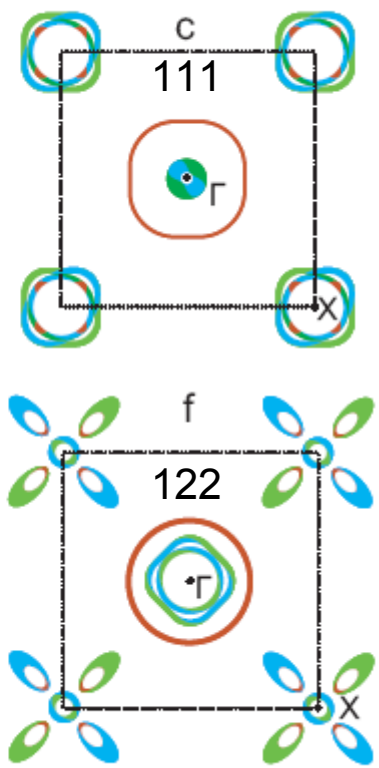
Table II: Coupling strength, $2\Delta/k_BT_c$, in iron-arsenic superconductors, as revealed by different experimental techniques — compare to the BSC universal value 3.53. Most of the available studies reveal two superconducting gaps of different magnitudes, which are represented in the table as "large" and "small". Refs. 2, 3, 4, 5, 6 are ARPES studies, Refs. 7, 8 are Andreev spectroscopy studies, Ref. 9 is a specific heat study.

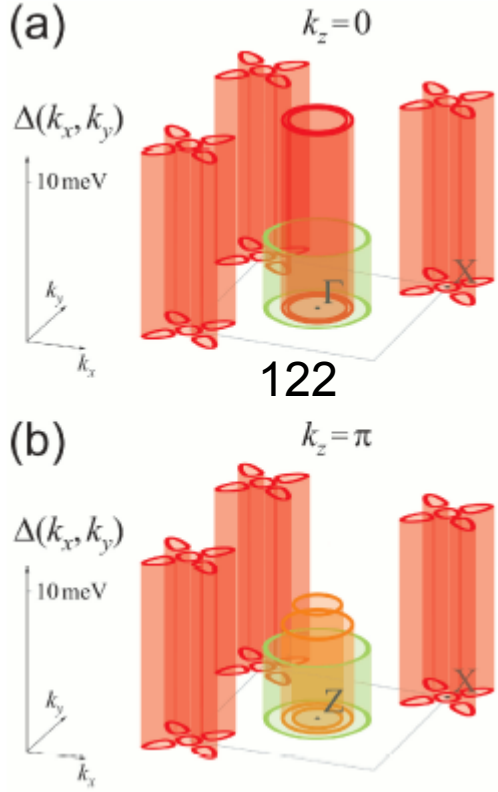
Iron based superconductors: magnetism, superconductivity and electronic structure (Review Article)

ArXiv:1209.0140

A. A. Kordyuk
Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine

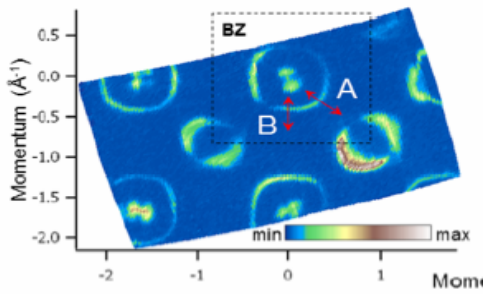


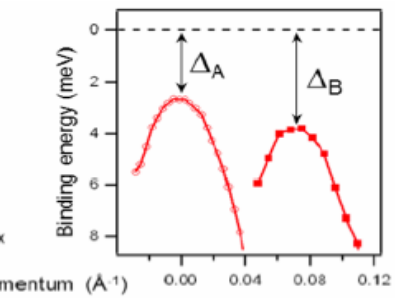


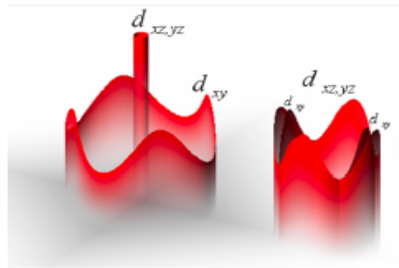


111

Spectra and Gaps in 122, 111

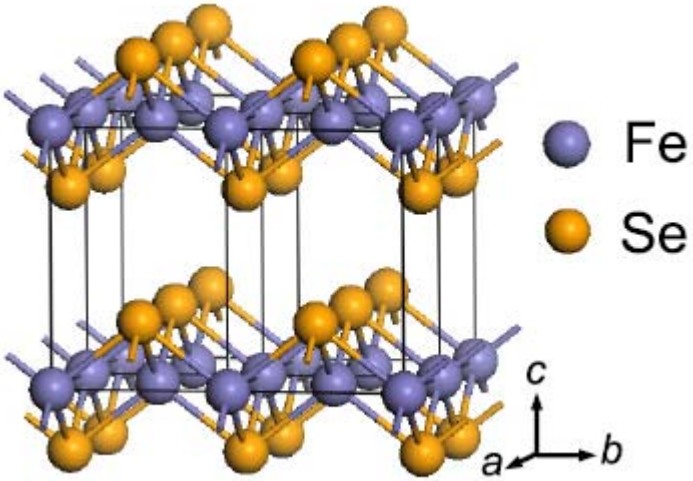


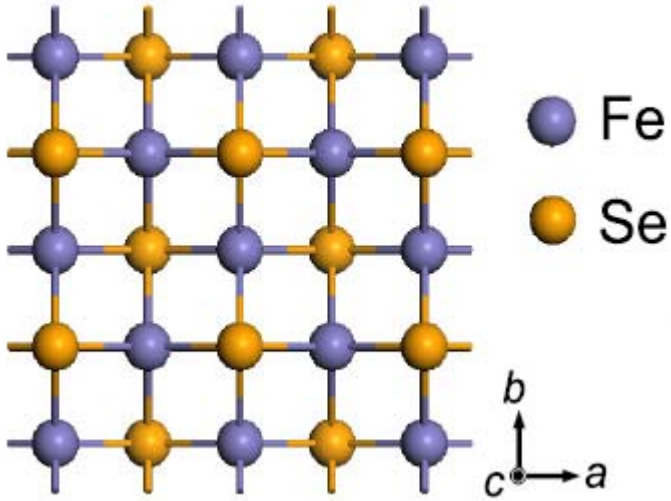




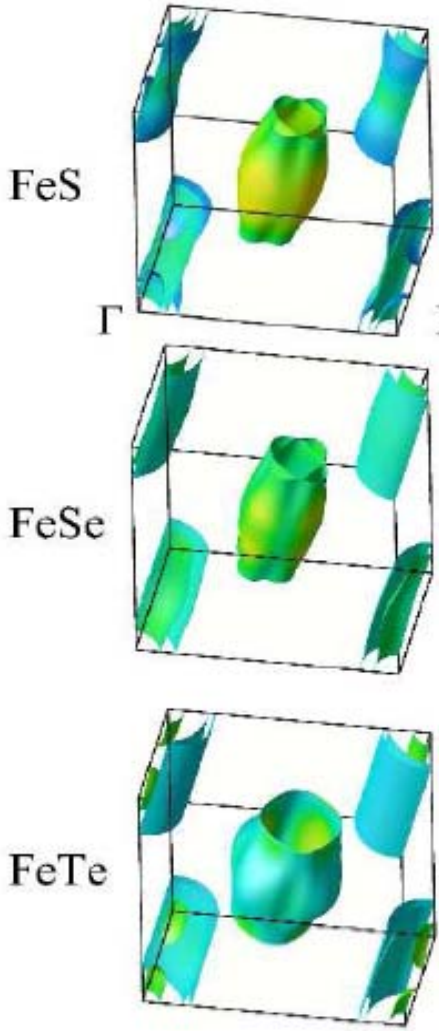
Superconductivity in the PbO-type Structure α–FeSe

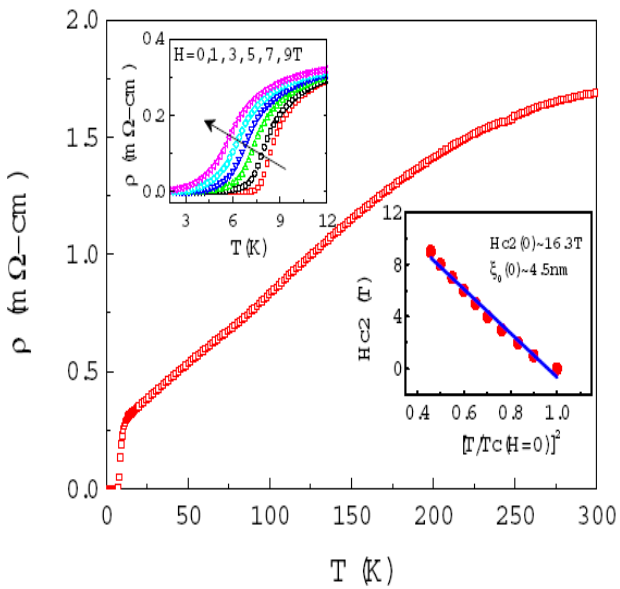
ArXiv: 0807.2369, 0807.4315, 0807.4775

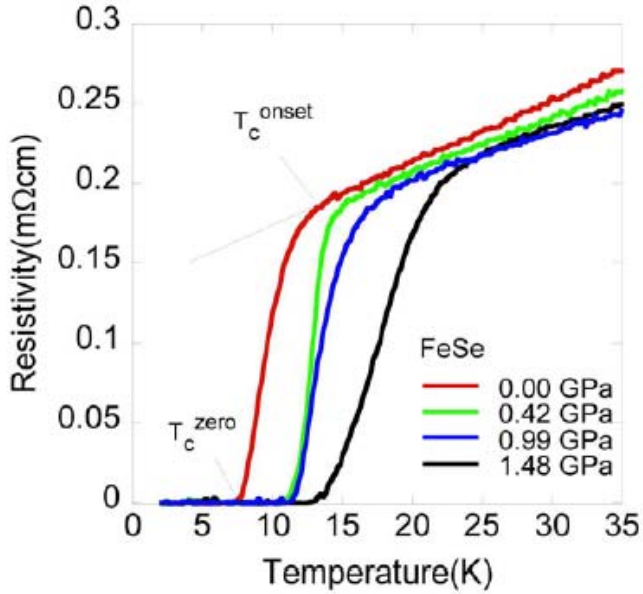




ArXiv:0807.4312





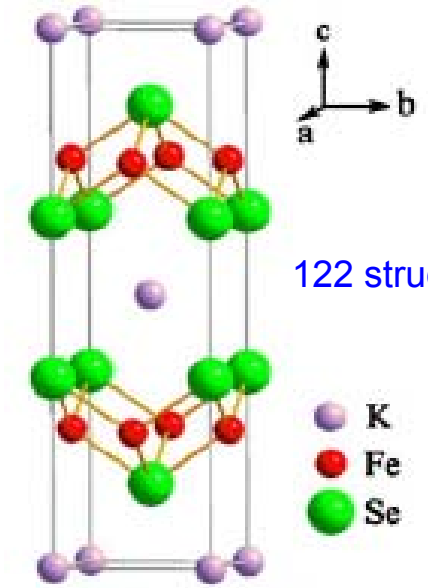


A(A=K,Cs,…)Fe2Se2: a New Class?

PHYSICAL REVIEW B 82, 180520(R) (2010)

Superconductivity in the iron selenide $K_xFe_2Se_2$ $(0 \leq x \leq 1.0)$

Jiangang Guo,[1] Shifeng Jin,[1] Gang Wang,[1] Shunchong Wang,[1] Kaixing Zhu,[1] Tingting Zhou,[1] Meng He,[2] and Xiaolong Chen[1]
[1]*Research & Development Center for Functional Crystals, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China*
[2]*National Centre for Nanoscience and Technology, Beijing 100190, China*
(Received 4 October 2010; revised manuscript received 11 November 2010; published 29 November 2010)



122 structure

$K_x^{+1}Fe^{+2}{}_2Se^{-2}{}_2$?

Vacancies?

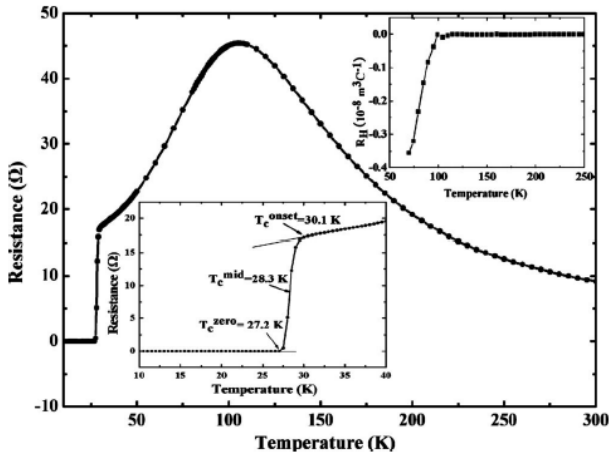


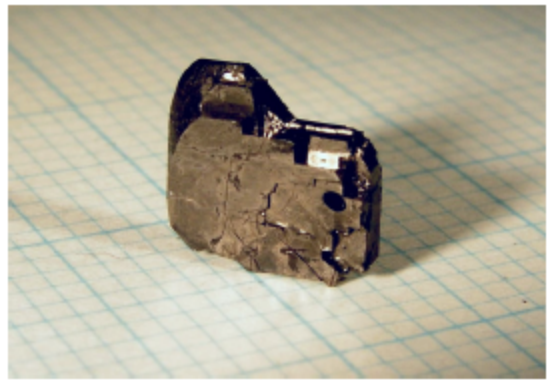
FIG. 3. The temperature dependence of electrical resistance for the $K_{0.8}Fe_2Se_2$ crystal sample. The lower inset shows the details of superconducting transition from 10 to 40 K. The upper inset shows temperature dependence of normal-state Hall coefficient for crystal sample.

Synthesis and crystal growth of $Cs_{0.8}(FeSe_{0.98})_2$: a new iron-based superconductor with T_c=27K

ArXiv: 1012.3637

A Krzton-Maziopa[1], Z Shermadini[2], E Pomjakushina[1], V Pomjakushin[3], M Bendele[2,4], A Amato[2], R Khasanov[2], H Luetkens[2] and K Conder[1]

$Cs_{0.8}(FeSe_{0.98})_2$



Pis'ma v ZhETF, vol. 93, iss. 3, pp. 182 – 185 © 2011 February 10

Electronic structure, topological phase transitions and superconductivity in $(K,Cs)_xFe_2Se_2$

I. A. Nekrasov[1)], *M. V. Sadovskii*[1)]

Institute for Electrophysics RAS, Ural Branch, 620016 Ekaterinburg, Russia

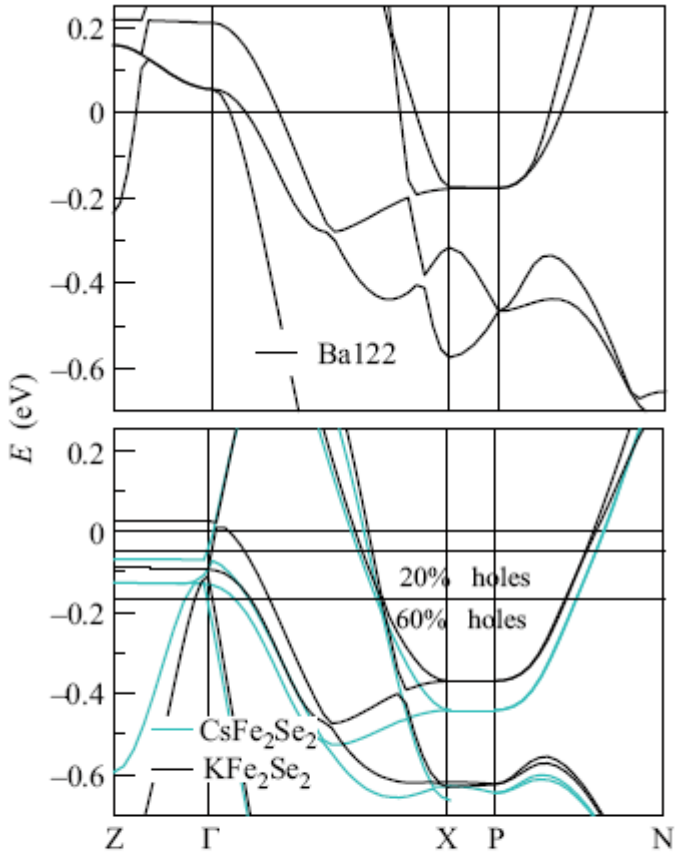
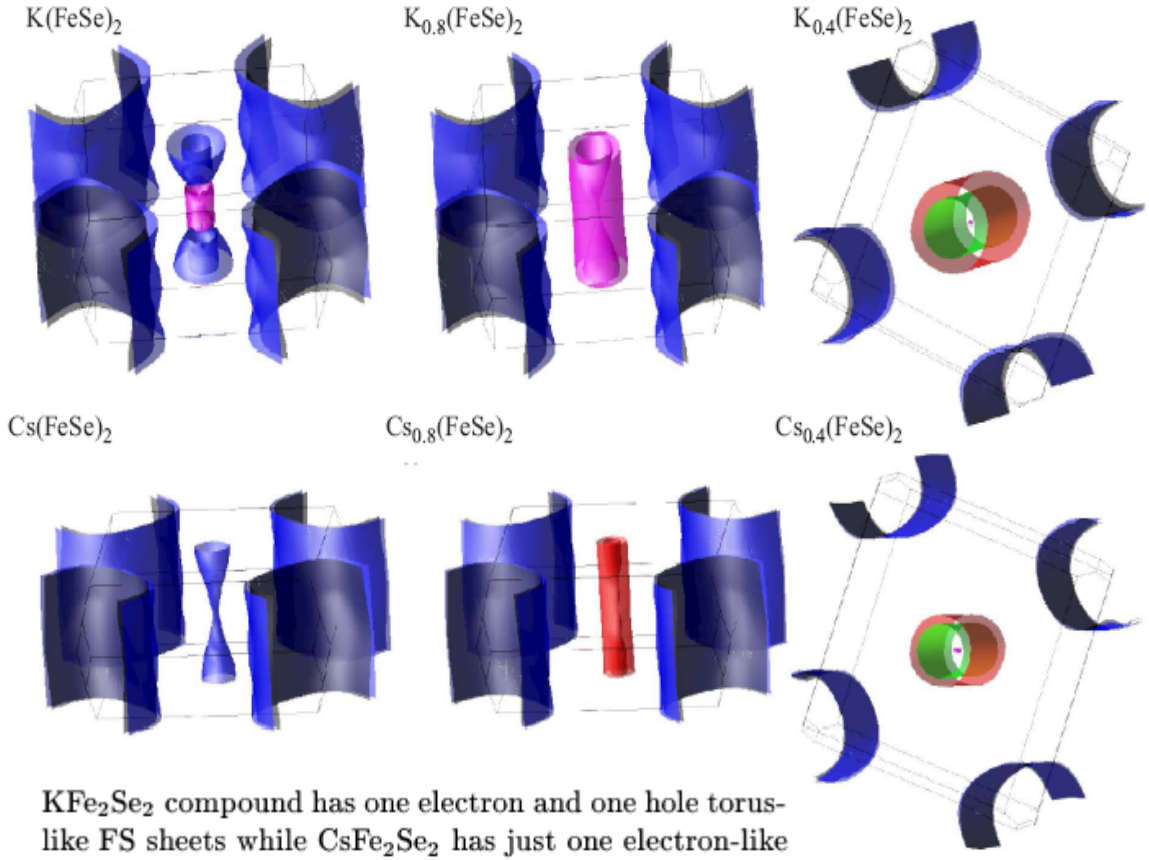


Fig.2. Top panel – LDA calculated band dispersions in the vicinity of the Fermi level for Ba122; Bottom panel – $K_xFe_2Se_2$ (black lines) and $Cs_xFe_2Se_2$ (gray lines). The Fermi level is at zero energy. Additional horizontal lines correspond to Fermi level position for the case of 20% and 60% hole doping



KFe_2Se_2 compound has one electron and one hole torus-like FS sheets while $CsFe_2Se_2$ has just one electron-like hourglass FS sheet. With hole doping KFe_2Se_2 torus transforms to electron-like hourglass and hole cylinder. For 20% hole doped Cs compound we get similar picture with smaller volume FS sheets of the same topology. For $x = 0.6$ both K and Cs new FeSe materials have Fermi surfaces quite similar to those in Ba122 iron pnictide

Common Fermi Surface Topology and Nodeless Superconducting Gap in $K_{0.68}Fe_{1.79}Se_2$ and $(Tl_{0.45}K_{0.34})Fe_{1.84}Se_2$ Superconductors Revealed from Angle-Resolved Photoemission Spectroscopy

ArXiv: 1102.1057

Lin Zhao[1], Daixiang Mou[1], Shanyu Liu[1], Xiaowen Jia[1], Junfeng He[1], Yingying Peng[1], Li Yu[1], Xu Liu[1], Guodong Liu[1], Shaolong He[1], Xiaoli Dong[1], Jun Zhang[1], J. B. He[2], D. M. Wang[2], G. F. Chen[2], J. G. Guo[1], X. L. Chen[1], Xiaoyang Wang[3], Qinjun Peng[3], Zhimin Wang[3], Shenjin Zhang[3], Feng Yang[3], Zuyan Xu[3], Chuangtian Chen[3] and X. J. Zhou[1,*]

[1] *Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[2] *Department of Physics, Renmin University of China, Beijing 100872, China*

[3] *Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, China*

(Dated: February 5, 2011)

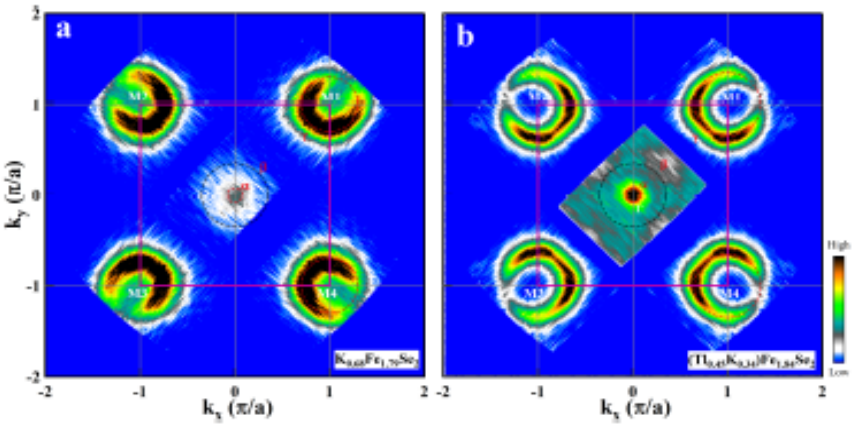


FIG. 1: Fermi surface mapping of $K_{0.68}Fe_{1.79}Se_2$ superconductor (T_c=32 K)(a) and $(Tl_{0.45}K_{0.34})Fe_{1.84}Se_2$ superconductor (T_c=28 K) (b) measured by using hν=21.2 eV light source. Near the M(π,π) point, one Fermi surface sheet is clearly observed which is marked as γ (for the sake of clarity, we refer the four equivalent M points in the first BZ as M1, M2, M3 and M4). Near the Γ(0,0) point, in addition to a tiny Fermi pocket observed which is marked as α, a weak large Fermi surface sheet (marked as β) is also discernable.

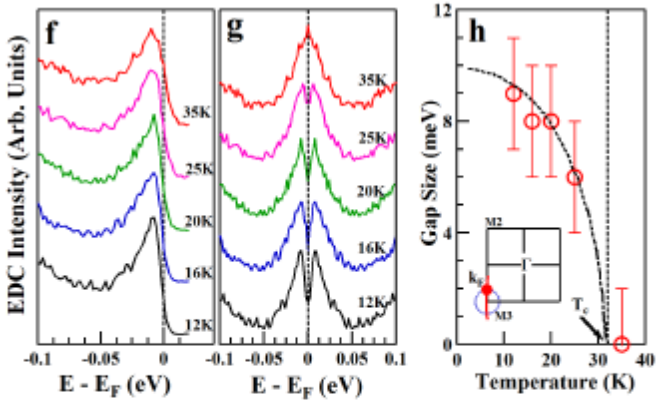
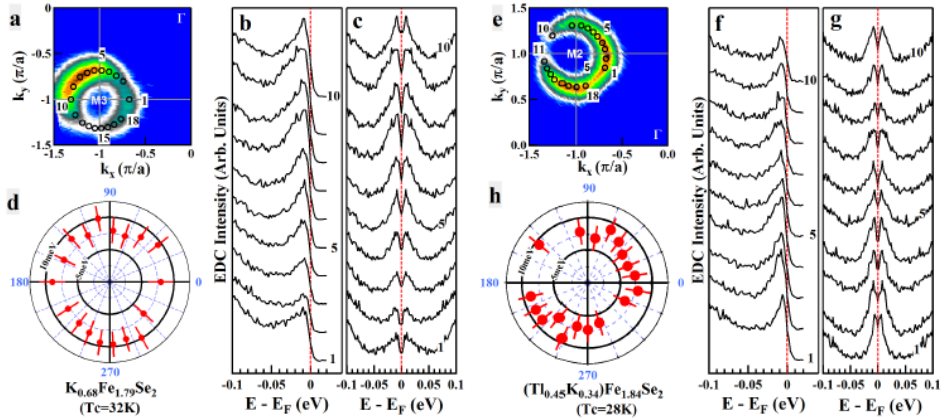


FIG. 3: Temperature dependence of the superconducting gap of $K_{0.68}Fe_{1.79}Se_2$ (T_c~32 K) along the γ Fermi pocket near M.

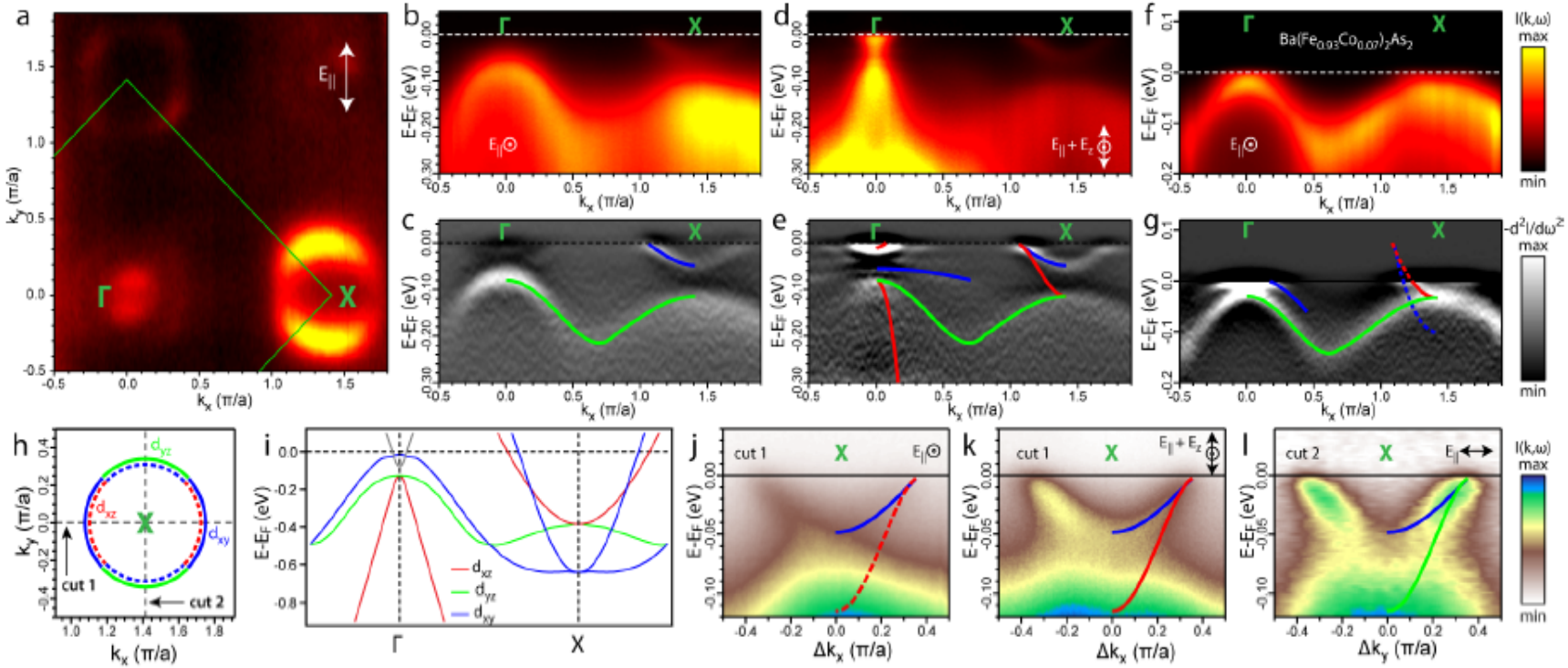


No nesting!

Observation of Temperature-Induced Crossover to an Orbital-Selective Mott Phase in $A_xFe_{2-y}Se_2$ (A=K, Rb) Superconductors

M. Yi,[1,2] D.H. Lu,[3] R. Yu,[4] S. C. Riggs,[1,2] J.-H. Chu,[1,2] B. Lv,[5] Z. Liu,[1,2] M. Lu,[1,6] Y.-T. Cui,[1]
M. Hashimoto,[3] S.-K. Mo,[7] Z. Hussain,[7] C. W. Chu,[5] I.R. Fisher,[1,2] Q. Si,[4] and Z.-X. Shen[1,2]

ArXiv:1208.5192



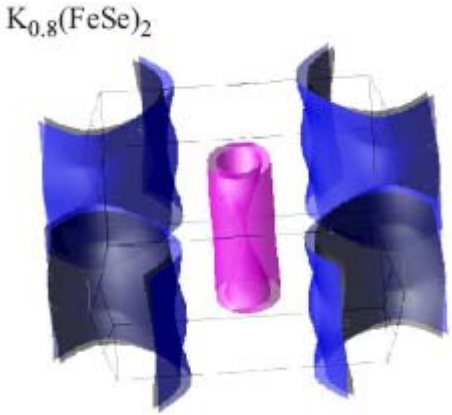
Measured electronic structure of $K_xFe_{2-y}Se_2$. (a) Fermi surface mapping by integrating 20meV window about E_F. Green lines outline the 2-Fe Brillouin zone. (b),(d) Spectral images and (c),(e) second derivatives taken along the Γ-X direction using light polarizations as marked. (f)-(g), equivalent of that of (b)-(c) for $Ba(Co_{0.07}Fe_{0.93})_2As_2$. (h) Schematic of the dominant orbital characters of the two electron pockets of the same size near X point, with one of the pockets (dotted) imploded for clarity. (i) LDA calculations [27] for KFS with the dominant orbital characters labeled. (j)-(l), Spectral images taken across the X-point under different polarizations and cut directions. Guides to eye for the observable bands are overlaid, with colors indicating the dominant orbital characters-blue: d_{xy}; red: d_{xz}; green: d_{yz}. All data taken at 30K, with 47.5eV photons except (d), (e), and (k), which were taken with 26eV photons.

$K_xFe_{2-y}Se_2$: LDA+DMFT Spectrum

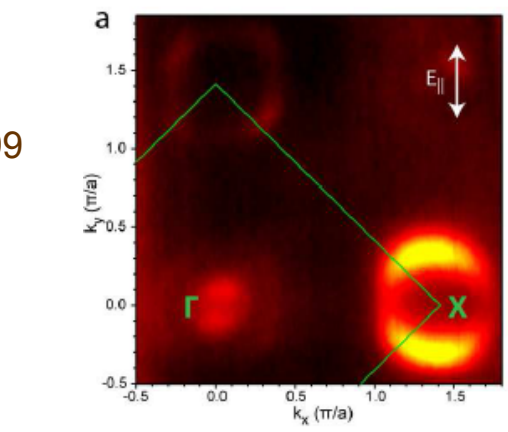
I.A.Nekrasov, N.S.Pavlov
M.V.Sadovskii, ArXiv:1211.3499

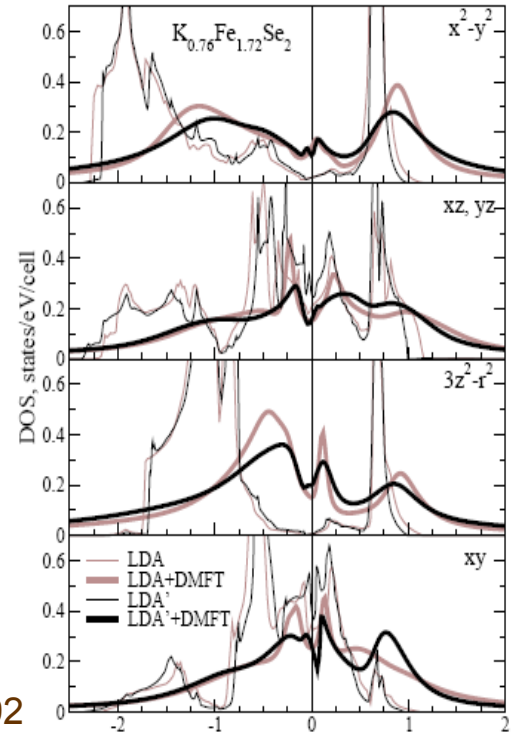
U=3.7 eV J=0.7eV
β=40

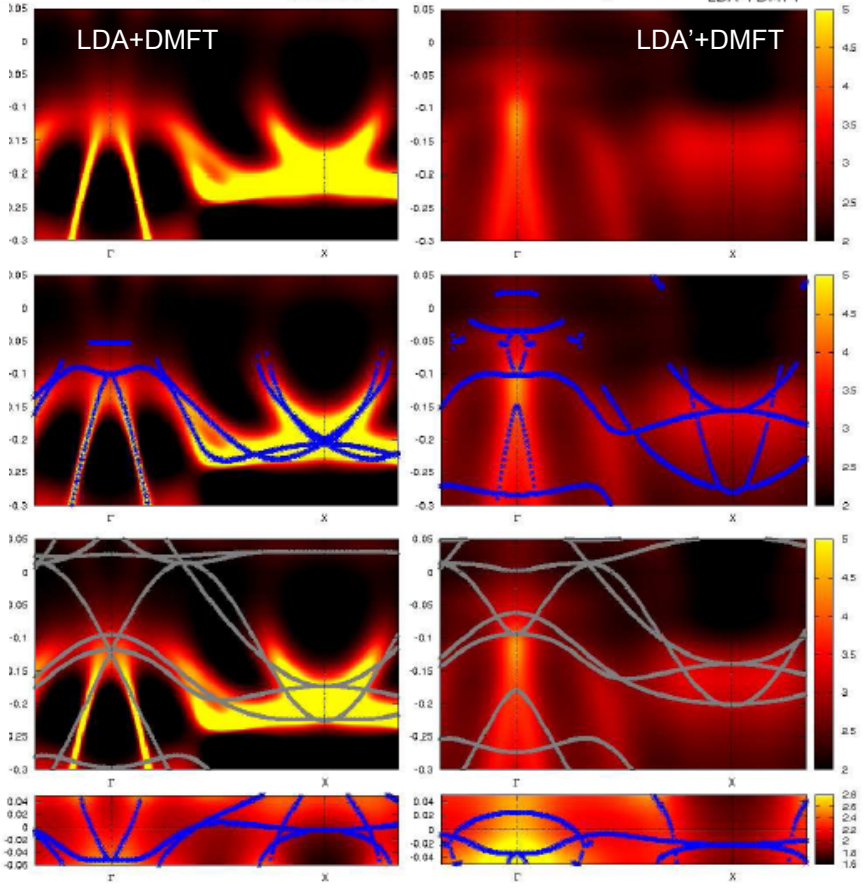
Correlations important!
LDA bands narrowing ~5
Strong damping near FS



ARPES dispersions:
Z.X.Shen et al. ArXiv:1208.5192

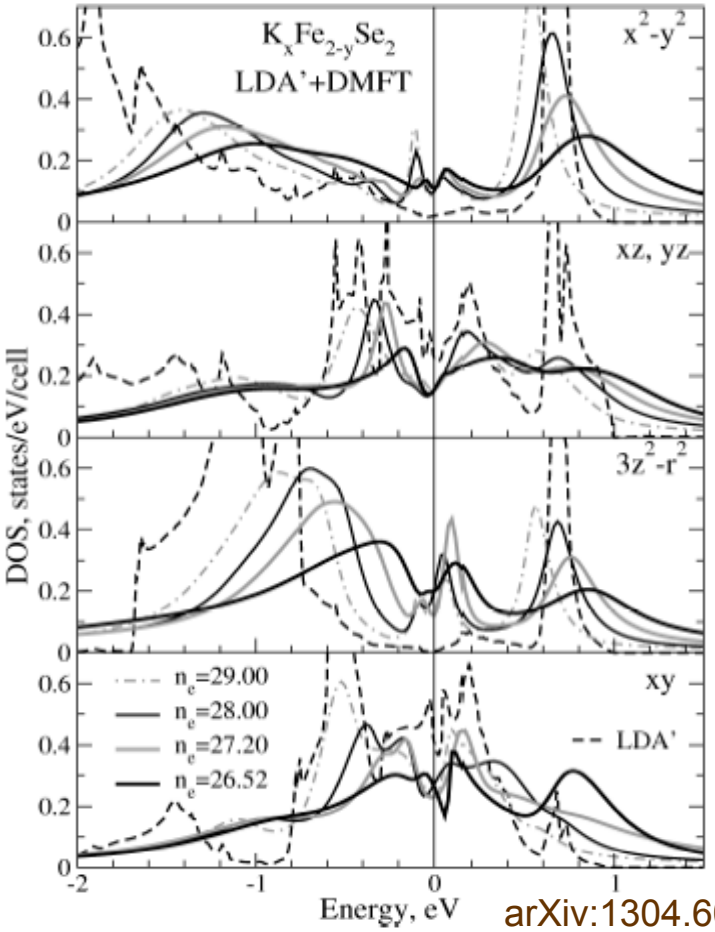






$K_{0.76}Fe_{1.72}Se_2$

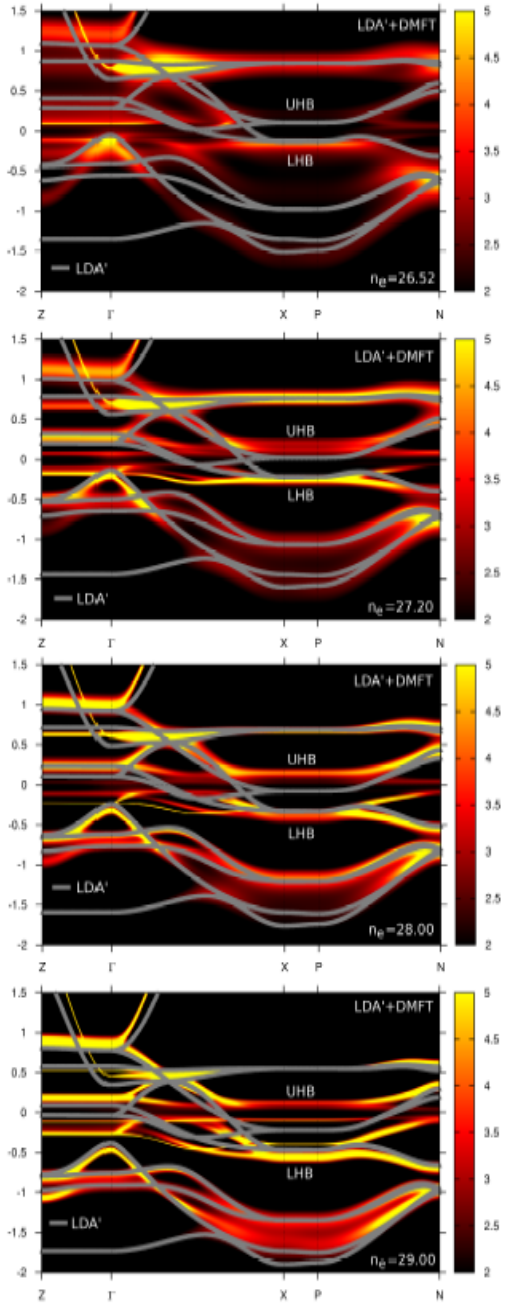
Doping $K_xFe_{2-y}Se_2$: LDA'+DMFT

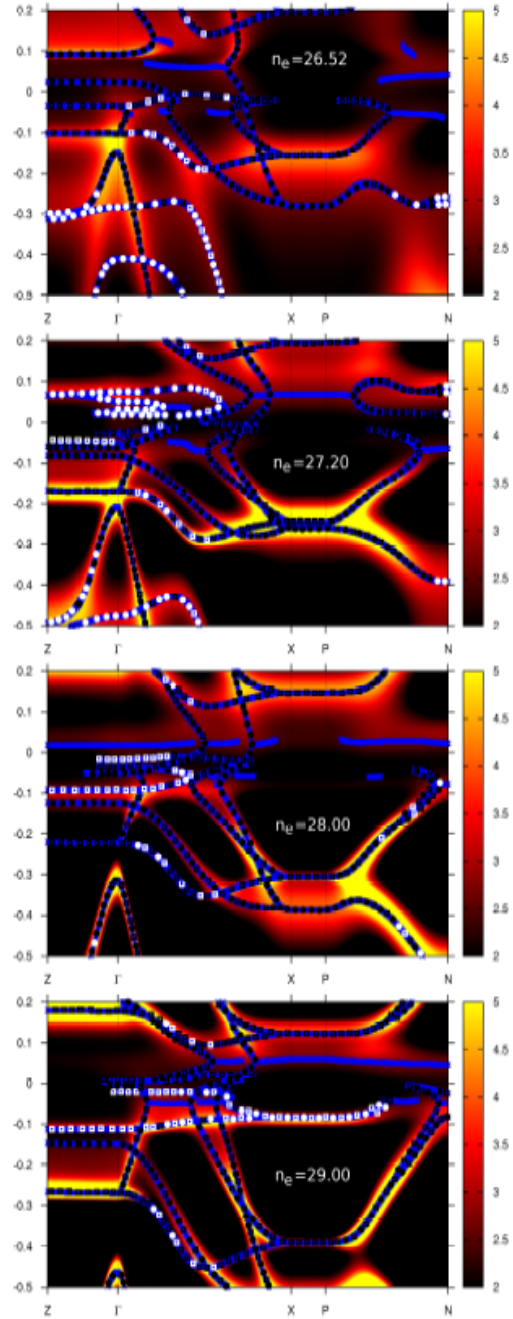


arXiv:1304.6030

TABLE I: Quasiparticle mass renormalization and energy shift (in eV, in round brackets) for different bare Fe-3d LDA′ orbitals for different hole doping levels n_e in the energy interval (-1.0;0.4).

Orbital chracter	n_e=26.52	n_e=27.20	n_e=28.00	n_e=29.00
xy	1.5 (-0.23)	3.9 (-0.73)	2.65 (-0.61)	1.7 (-0.35)
xz,yz (1)	4.2 (-0.78)	3.0 (-0.75)	2.6 (-0.69)	1.7 (-0.38)
xz,yz (2)	2.3 (-0.48)	2.5 (-0.60)	2.6 (-0.69)	1.7 (-0.38)
xy,xz,yz	1.2 (-0.10)	1.3 (-0.10)	1.3 (-0.10)	1.4 (-0.17)
$3z^2$-r^2 (1)	4.7 (-0.85)	2.0 (-0.30)	1.3 (-0.03)	1.25 (0.0)





A(A=K,Cs,…)Fe2Se2: a New AFM Superconductor

A Novel Large Moment Antiferromagnetic Order in $K_{0.8}Fe_{1.6}Se_2$ Superconductor

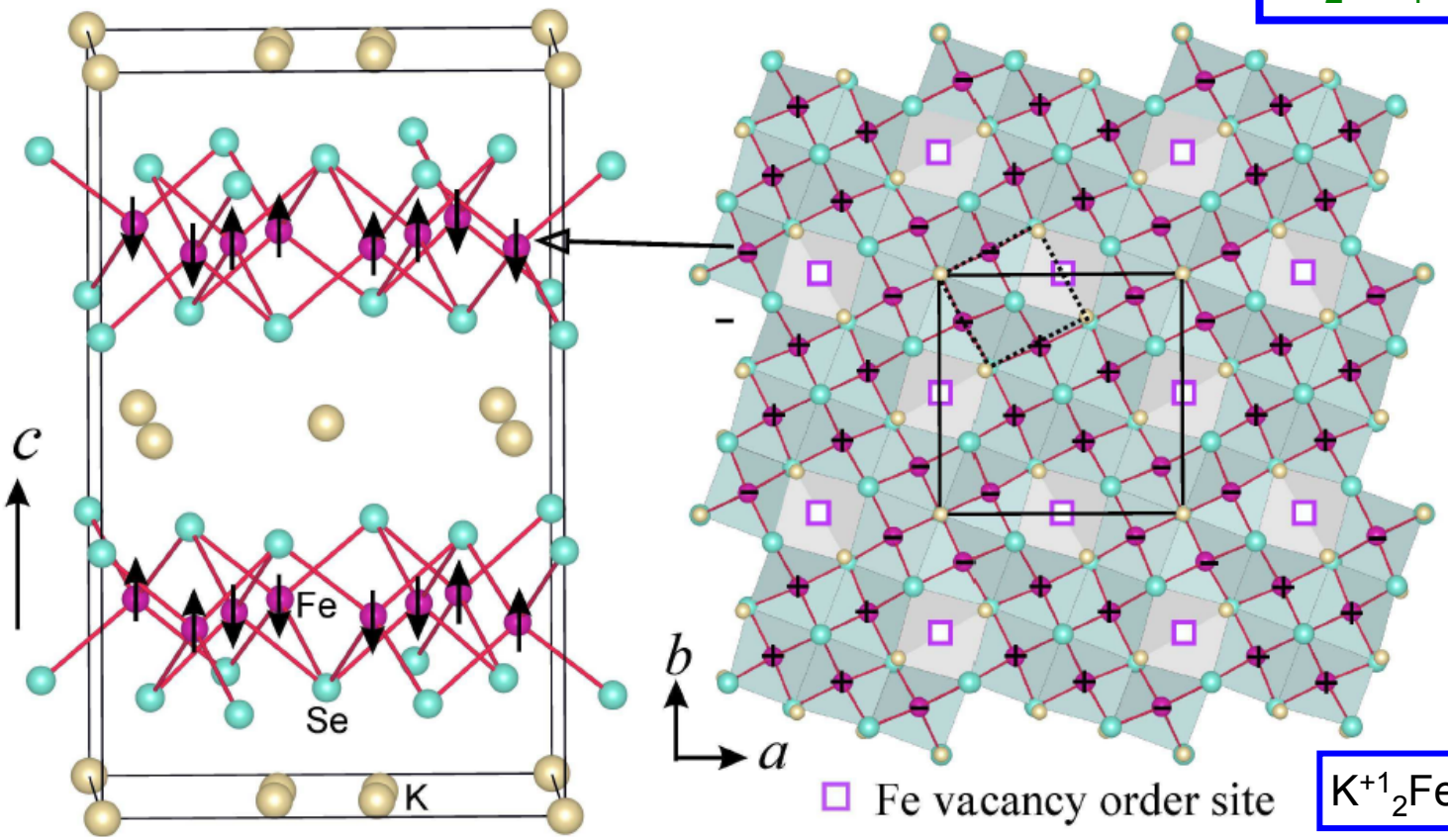
Wei Bao,[1,*] Q. Huang,[2] G. F. Chen,[1] M. A. Green,[2,3] D. M. Wang,[1] J. B. He,[1] X. Q. Wang,[1] and Y. Qiu[2,3]

[1] *Department of Physics, Renmin University of China, Beijing 100872, China*
[2] *NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA*
[3] *Dept. of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA*

(Dated: February 7, 2011)

ArXiv: 1102.0830

$K_2Fe_4Se_5$?

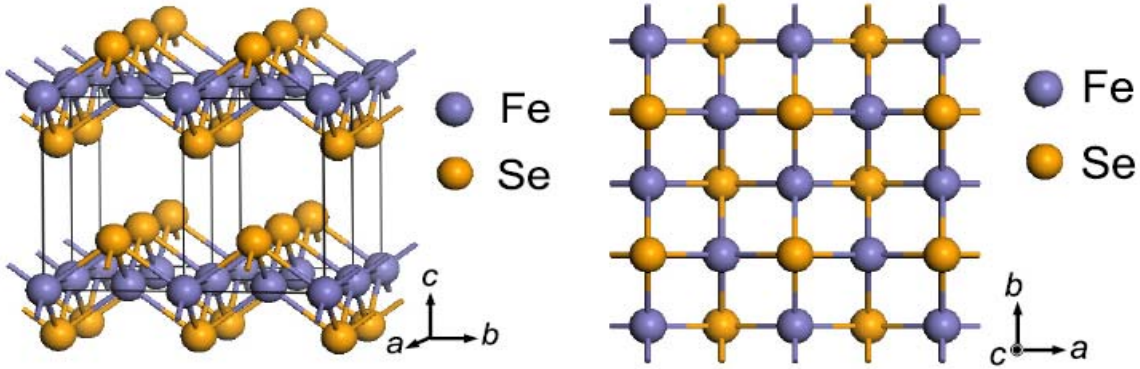


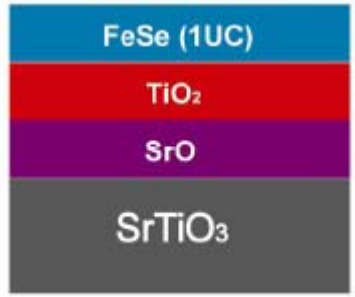
$K^{+1}{}_2Fe^{+2}{}_4Se^{-2}{}_5$!

The superconducting composition is identified as the iron vacancy ordered $K_{0.8}Fe_{1.6}Se_2$ with T_c above 30 K. A novel large moment 3.31 μ_B/Fe antiferromagnetic order which conforms to the tetragonal crystal symmetry has the unprecedentedly high an ordering temperature $T_N \approx 559$ K for a bulk superconductor.

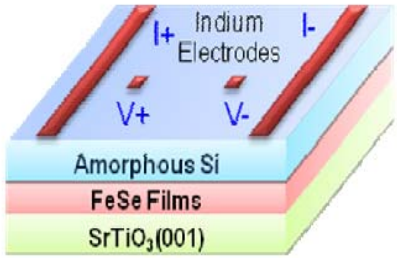
Interface induced high temperature superconductivity in single unit-cell FeSe films on $SrTiO_3$

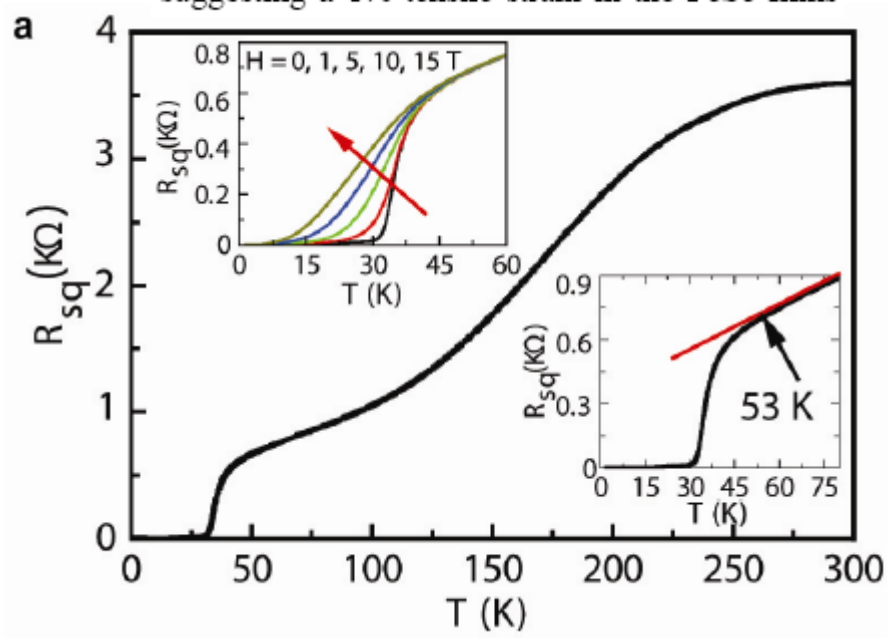
ArXiv:1201.5694

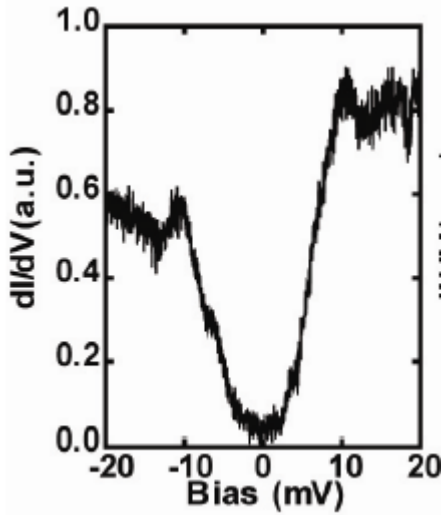




The in-plane lattice constant is 3.8 Å, suggesting a 1% tensile strain in the FeSe films





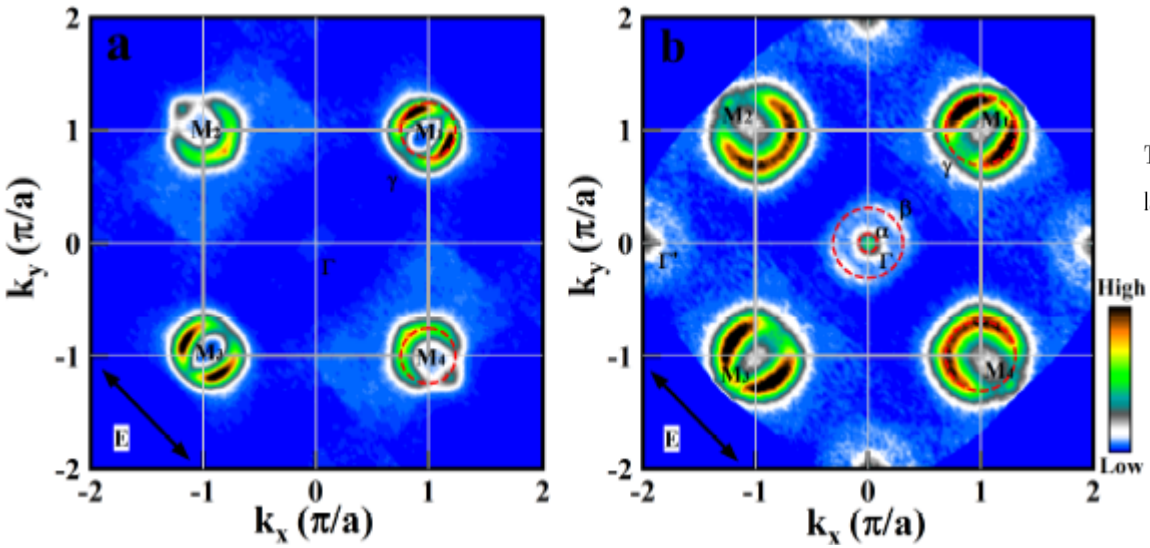


Electronic Origin of High Temperature Superconductivity in Single-Layer FeSe Superconductor

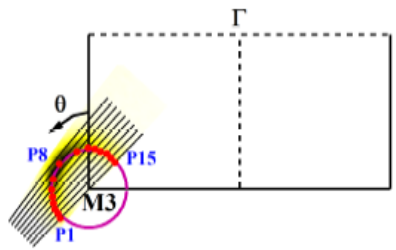
ArXiv:1202.5849

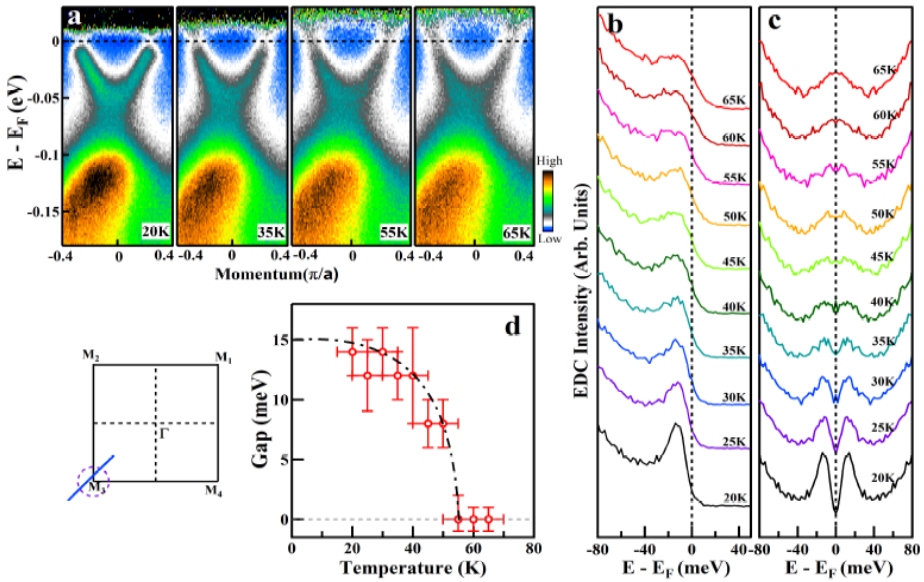
single layer FeSe

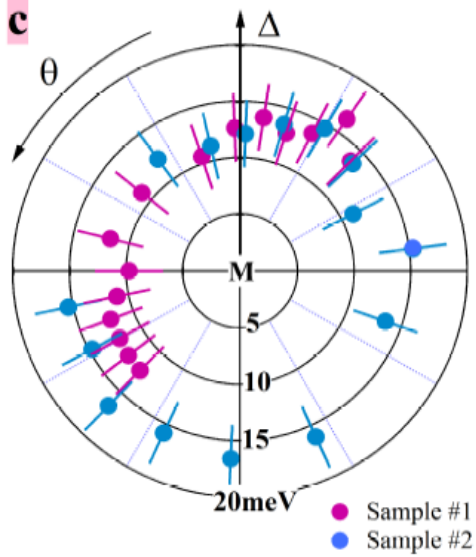
$(Tl_{0.58}Rb_{0.42})Fe_{1.72}Se_2$ superconductor (T_c=32 K)



The T_c is still unusually high even considering the newly-discovered intercalated FeSe system $A_xFe_{2-y}Se_2$ (A=K, Cs, Rb and Tl) with a T_c at 32 K

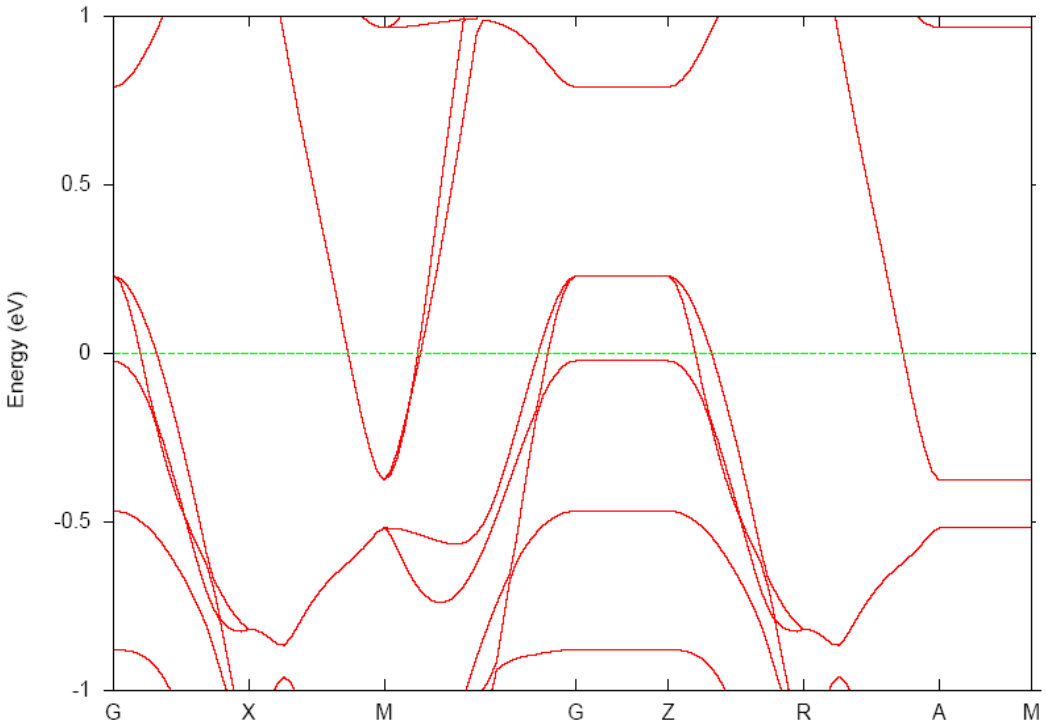


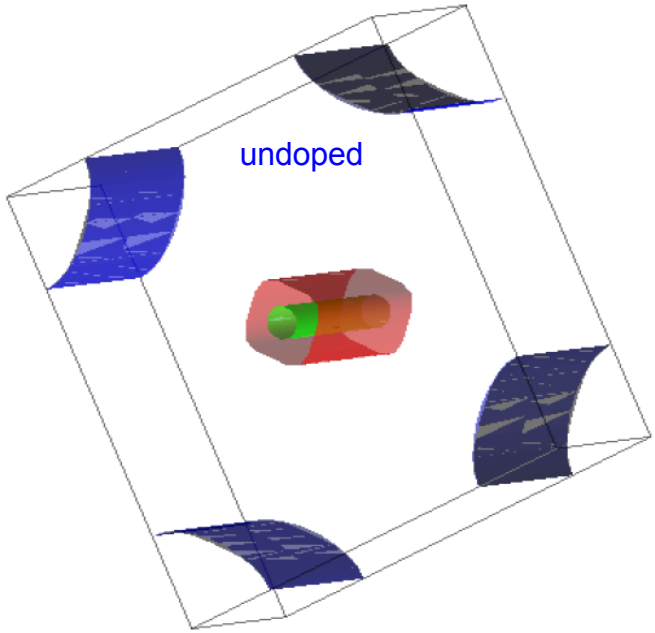


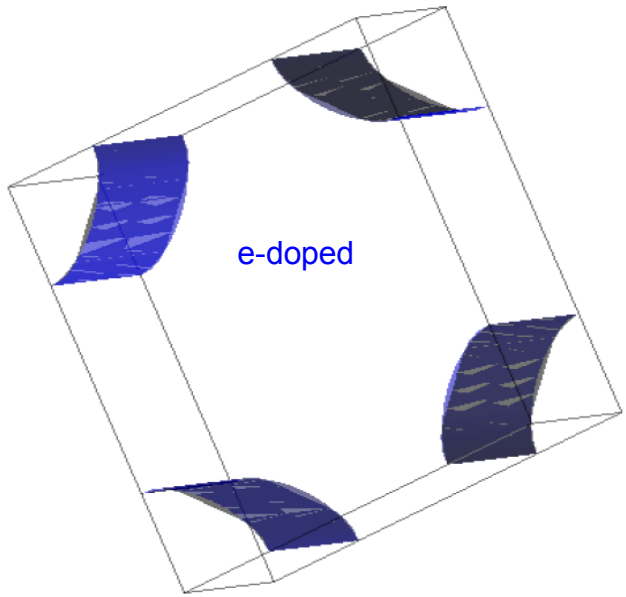


LDA in single layer FeSe

I.A. Nekrasov (unpublished)



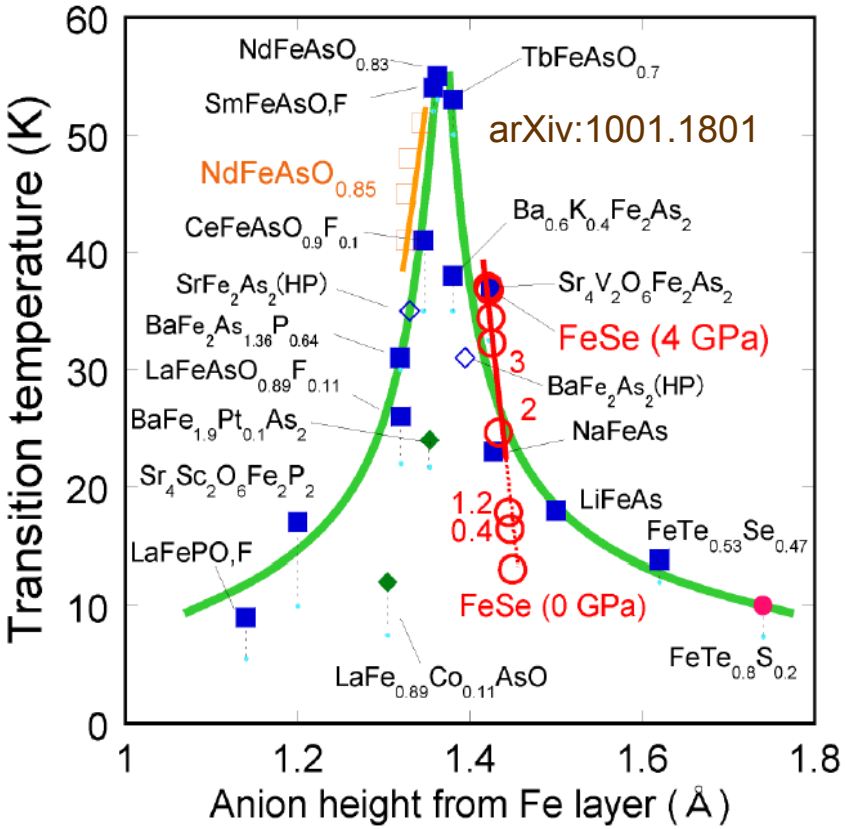


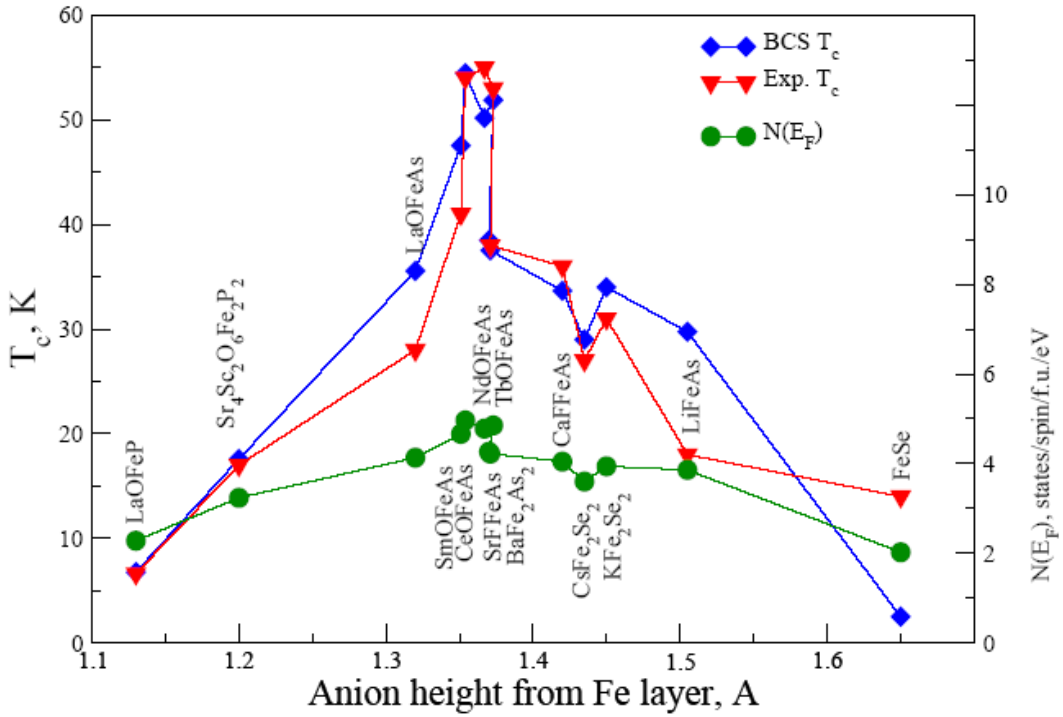


Self – doping at the interface?

E_F shift ~ +0.25 eV (or 0.2 electron per Fe)

Tc and Density of States Correlation





System	Δz_a, Å	N(E_F), states/cell/eV	T_c^{BCS}, K	T_c^{exp}, K
LaOFeP	1.130	2.28	3.2	6.6
$Sr_4Sc_2O_6Fe_2P_2$	1.200	3.24	19	17
LaOFeAs	1.320	4.13	36	28
SmOFeAs	1.354	4.96	54	54
CeOFeAs	1.351	4.66	48	41
NdOFeAs	1.367	4.78	50	53
TbOFeAs	1.373	4.85	52	54
SrFFeAs	1.370	4.26	38	36
$BaFe_2As_2$	1.371	4.22	38	38
CaFFeAs	1.420	4.04	34	36
$CsFe_2Se_2$	1.435	3.6	29	27
KFe_2Se_2	1.45	3.94	34	31
LiFeAs	1.505	3.86	31	18
FeSe	1.650	2.02	3	14

arXiv: 1004.0801

The Δz_a dependence of N(E_F) inevitably leads to the corresponding dependence of superconducting critical temperature T_c. To estimate this we, first of all, use the elementary BCS expression: $T_c = 1.14\omega_D e^{-1/\lambda}$, where ω_D is the characteristic frequency of collective excitations involved in pairing interaction (phonons, spin fluctuations etc.), and $\lambda = gN(E_F)/2$ is the dimensionless pairing interaction constant (g is the appropriate dimensional coupling constant). In the following we take ω_D=350 K in rough accord with neutron scattering experiments on phonon density of states for La111

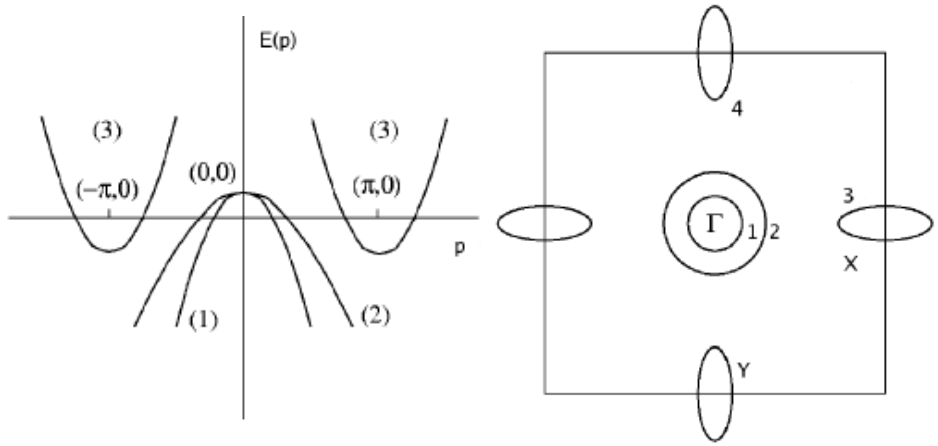
Simple model of multiple – band superconductivity

V. Barzykin, L.P. Gorkov. Pis'ma ZhETF 88, 142 (2008); arXiv: 0806.1993

$$\Delta_i(p) = T\sum_{j;\omega_n}\int V^{i,j}(p-p')dp' F_j(\omega_n, p')$$

Δ_i, ν_i - a superconducting gap and DOS on the *i*-th sheet of the Fermi surface

$$V = \begin{pmatrix} u & w & t & t \\ w & u' & t & t \\ t & t & \lambda & \mu \\ t & t & \mu & \lambda \end{pmatrix}$$



Schematic electronic spectrum and Fermi surfaces of FeAs superconductor in the extended band picture.

$V^{i,j}$ - intraband and interband pairing coupling constants matrix.

$\lambda = V^{eX,eX} = V^{eY,eY}$ - pairing interactions on the same electronic pockets at point *X* or *Y*,

$\mu = V^{eX,eY}$ - connects electrons of different electronic pockets,

$u = V^{h1,h1}$, $u' = V^{h2,h2}$, $w = V^{h1,h2}$ - BCS interactions within two hole-like pockets,

$t = V^{h,eX} = V^{h,eY}$ - couple electrons at points *X* and *Γ*.

$$\Delta_i = -\sum_j V^{i,j}\nu_j\Delta_j \ln\frac{2\gamma\omega_c}{\pi T_c}$$

$$T_c = \frac{2\gamma\omega_c}{\pi} e^{-1/g_{eff}}$$

$1/g_{eff}$

! H.Suhl, B.Matthias, L.Walker
Phys.Rev.Lett. 3, 552 (1959)
V.Moskalenko FMM 4, 503 (1959)

$$g_{eff}\Delta_i = \sum_j g_{ij}\Delta_j$$

E. Z. Kuchinskii[1)], M. V. Sadovskii[1)]

Pis'ma v ZhETF, vol. 89, iss. 3, pp. 176 – 180

arXiv: 0901.0164

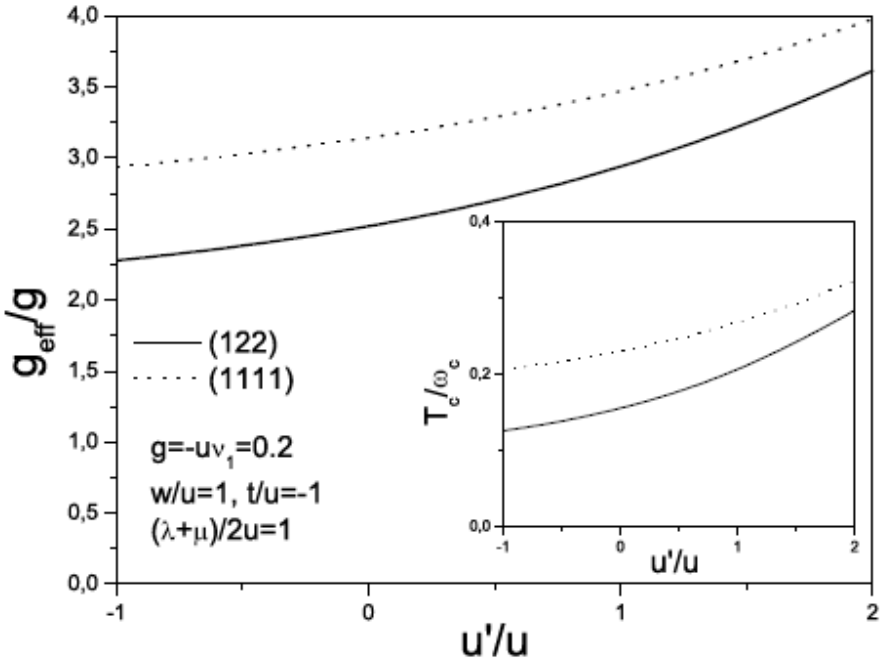
$$g_{ij} \equiv -V^{i,j}\nu_j$$

Matrix of dimensionless coupling constants

$$Det(g_{ij} - g_{eff}\delta_{ij}) = 0$$

Secular equation, physical solution corresponds to a maximal positive value of g_{eff}, which determines the highest value of T_c

Effective coupling – from weak to strong?



! **Effective coupling constant g_{eff} is significantly larger than the pairing constant g on the small hole - like cylinder**. It can be said that coupling constants from different cylinders effectively produce "additive" effect. In fact this can lead to high enough values of T_c even for relatively small values of intraband and interband pairing constants.

- $g_{eff}, T_c\,(d_{x^2-y^2}\text{ pairing}) < g_{eff}, T_c\,(s^{\pm}\text{ pairing})$

Value of T_c in multiple bands systems is determined by the **relations between partial densities of states** (and pairing constants) on different sheets of the Fermi surface, **not only by the total density of states** at the Fermi level.

1. No interband pairing

$$\hat{g} = \begin{pmatrix} g_1 & 0 & 0 & 0 \\ 0 & g_2 & 0 & 0 \\ 0 & 0 & g_3 & 0 \\ 0 & 0 & 0 & g_4 \end{pmatrix} \longrightarrow g_{eff} = max(g_i)$$

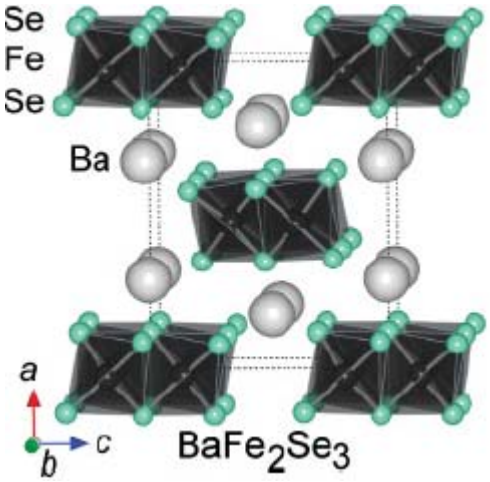
2. All pairing interactions (both intraband and interband) are just the same - u, and all partial densities of states on all four Fermi surface pockets are also the same - ν_1.

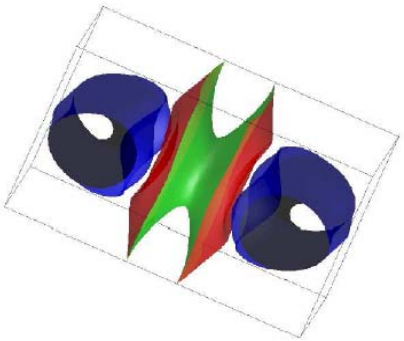
$$\hat{g} = -u\nu_1 \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \longrightarrow g_{eff} = 4g = -4u\nu_1$$

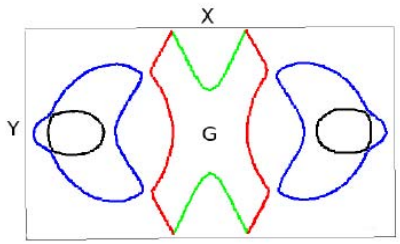
Is there a nontrivial "optimal" band structure (number of bands etc.)?

Ba 123 FeSe

$Ba^{+2}(Fe^{+2})_2(Se^{-2})_3$





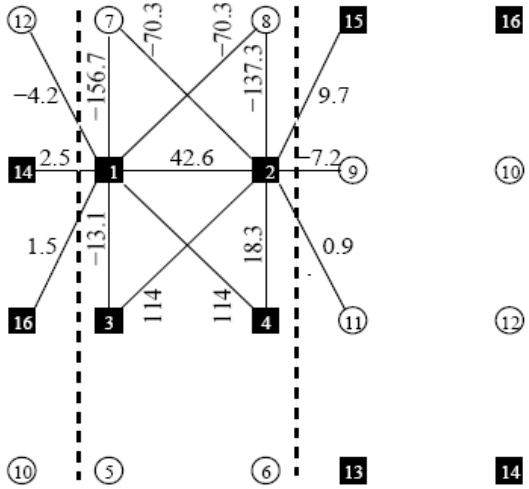


Electronic and Magnetic Structure of Possible Iron Based Superconductor $BaFe_2Se_3$

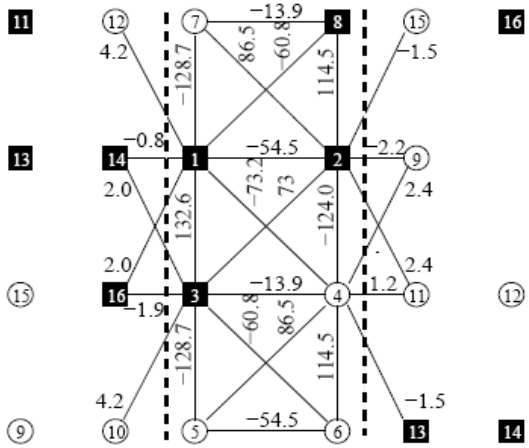
ArXiv: 1111.7046

[a]M. V. Medvedev, [b]I. A. Nekrasov, [a,b]M. V. Sadovskii[1)]

τ_1 spin configuration of Ba123 ("plaquettes")



τ_2 spin configuration of Ba123 ("zigzags")



In case of magnetic structure with several collinear magnetic sublattices Heisenberg model Hamiltonian for classical spin vectors can be written as:

$$H = -\frac{1}{2}\sum_{i,n\neq j,m} I_{i,n,j,m}\vec{S}_{i,n}\vec{S}_{j,m} = \\ = -\frac{1}{2}\sum_{i,n\neq j,m} I_{i,n,j,m}S^2\vec{e}_{i,n}\vec{e}_{j,m}, \qquad (1)$$

where $I_{i,n,j,m}$ is exchange integral between site i of sublattice n and site j of sublattice m, S – classical spin vector length and $\vec{e}_{i,n}$ is the unit vector of spin direction. Self-consistent equations for thermodynamic averages of spin z-projections $\sigma_{in} \equiv < S^z_{i,n} >$ within mean-field approach can be linearized near Neel temperature T_N and written as:

$$T_N\sigma_{in} = \frac{S^3}{3}\sum_{jm} I_{in,jm}\sigma_{jm}. \qquad (2)$$

Due to translation invariance of the crystal the values of $\sigma_{in} = \sigma_n$ are independent of site number in magnetic sublattice. Then Neel temperature T_N is determined by the solution of the full system of linear equations for σ_n for all magnetic sublattices.

Employing the calculated values of exchange parameters given (in K) in Fig. 4, together with calculated value of magnetic moment on iron $\mu_{Fe} = 2.55\mu_B$ (corresponding classical spin vector value S=1.275), one can get from Eqs. (5) and (6) the Neel temperature $T_N(\tau_1)$=217K, which is quite close to the experimental value of T_N^{exp} ~250K.

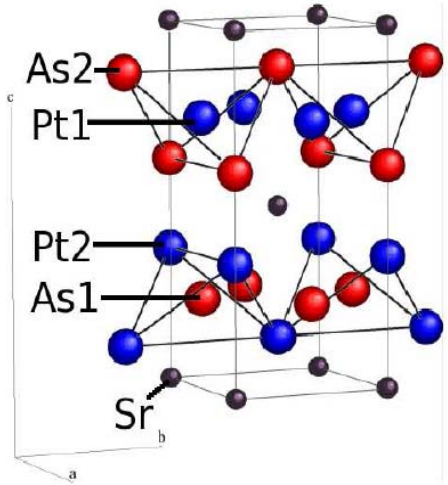
$SrPt_2As_2$

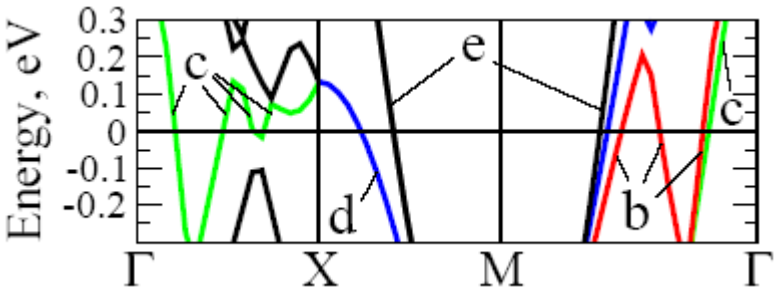
Pis'ma v ZhETF, vol. 92, iss. 11, pp. 833 – 836

Electronic structure of novel multiple-band superconductor $SrPt_2As_2$

I. A. Nekrasov[1)], *M. V. Sadovskii*[1)]

ArXiv: 1011.1746





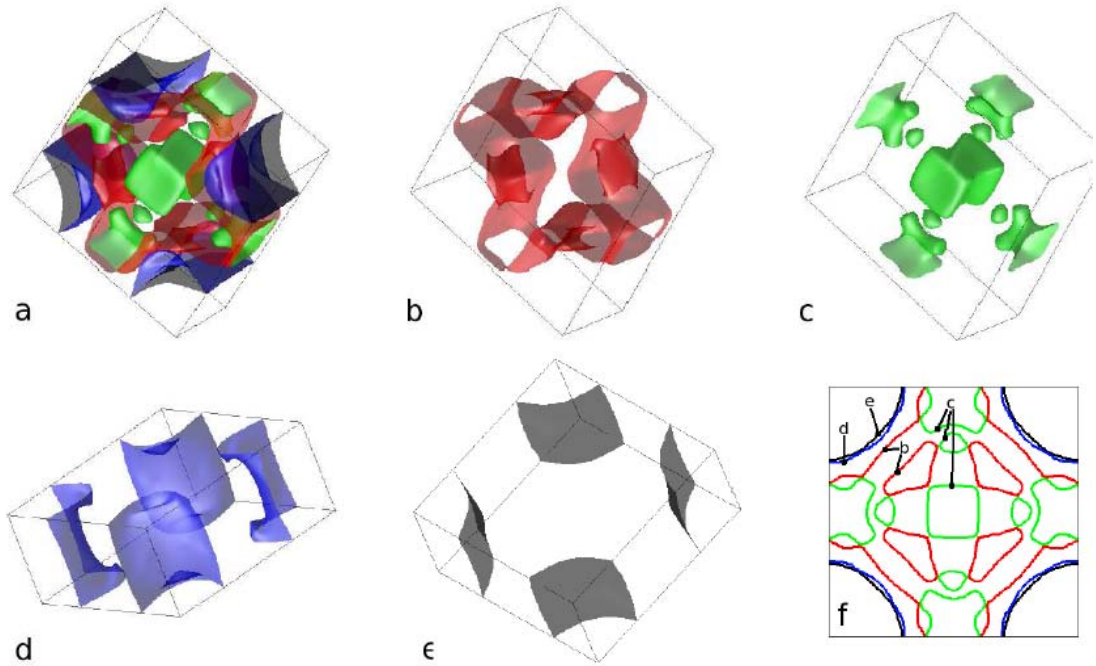


Fig. 4. LDA calculated FS for $SrPt_2As_2$. a – all FS sheets together; b,c,d,e – separate view of each of four FS sheets. Among these (b) is electron-like, (c) is hole-like and (d) and (e) are electron-like. f – crossection of FS at k_z=0 with color coding corresponding to Fermi sheets b,c,d and e.

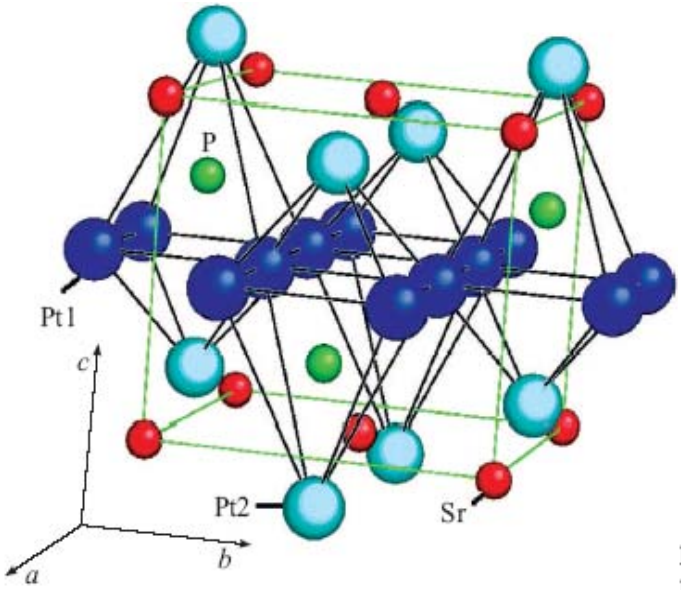
APt_3P (A=Ca,Sr,La)

Pis'ma v ZhETF, vol. 96, iss. 4, pp. 243 – 246

Electronic structure of new multiple band Pt-pnictide superconductors APt_3P

ArXiv: 1205.5387

I. A. Nekrasov[+1), *M. V. Sadovskii*[+*1)



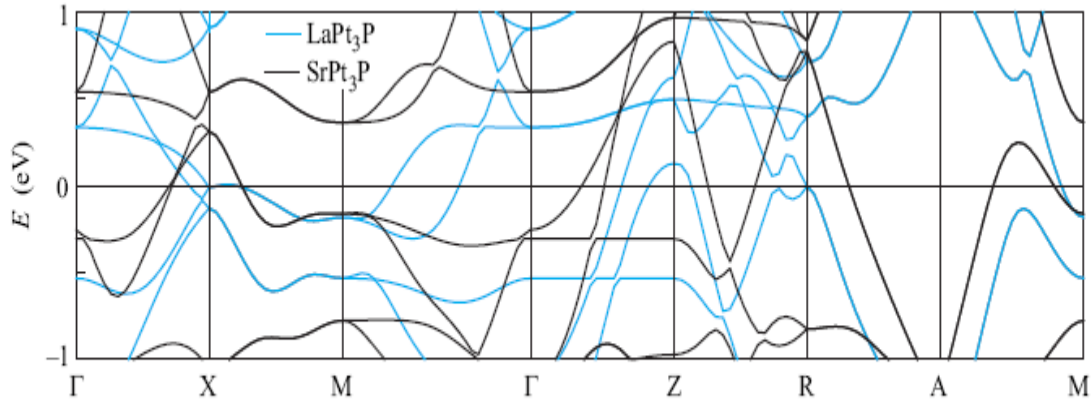


Fig. 3. LDA calculated band dispersions in the vicinity of the Fermi level for $SrPt_3P$ (black line) and $LaPt_3P$ (gray line). Fermi level is at zero energy

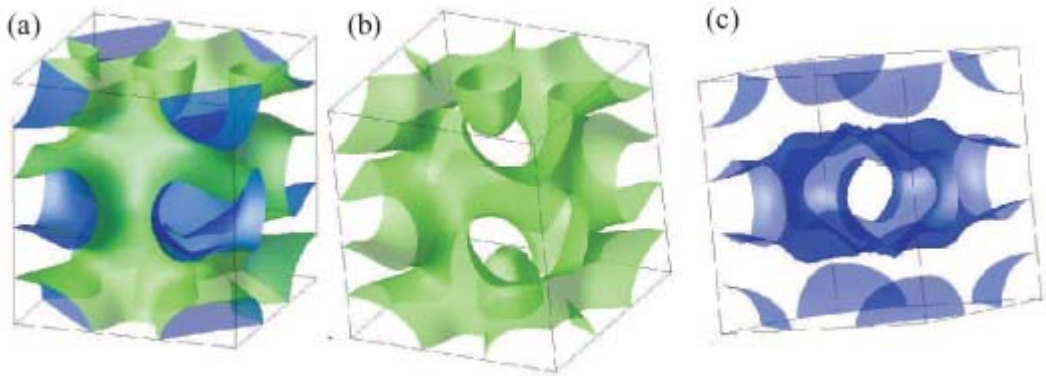


Fig. 4. LDA calculated Fermi surface for $SrPt_3P$ (a) and its separate sheets (b, c)

As simple BCS expression for T_c is probably too crude, we also used the McMillan expression [19]:

$$T_c = \frac{\omega_D}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right], \qquad (1)$$

where μ^* is the Coulomb pseudopotential. Quite similar results were also obtained with Allen-Dynes formula [20], considered to be the best interpolation expression for T_c in strongly coupled superconductors. Taking the "optimistic" value of Coulomb pseudopotential $\mu^* = 0$, we repeat our previous analysis. Now Eq. (1) gives $\lambda = 0.61$ for $SrPt_3P$ and corresponding $T_c = 5.6\,K$ for $LaPt_3P$. Once we assume more typical value of $\mu^* = 0.1$, we get $\lambda = 0.85$ for $SrPt_3P$ and then $T_c = 5.4\,K$ for La compound is obtained.

$Sr(Ca,Ba)Pd_2As_2$

Comparative Study of Electronic structure of New Superconductors $(Sr,Ca)Pd_2As_2$ and related compound $BaPd_2As_2$.

[a]I. A. Nekrasov[1)], [a,b]M. V. Sadovskii[2)]

ArXiv: 1305.3979

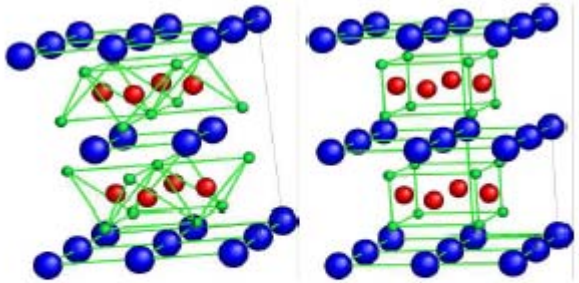


Fig. 1. Crystal structure of $(Sr,Ca)Pd_2As_2$ (left) and $BaPd_2As_2$ (right). Blue balls are Sr,Ba ions, green – As and red – Pd.

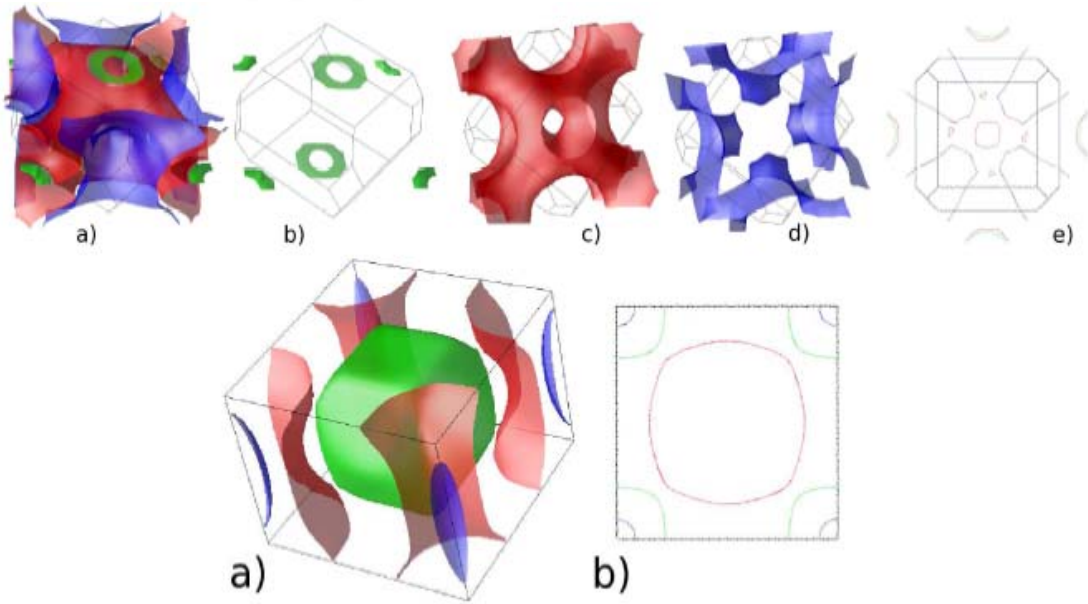


Fig. 4. LDA calculated FS for $(Sr,Ca)Pd_2As_2$ (top) and $BaPd_2As_2$ (bottom). a – all FS sheets together for both systems; b,c,d (top panel) – separate view of each of three FS sheets for $(Sr,Ca)Pd_2As_2$; e (top panel) and b (lower panel) – crossection of FS at k_z=0 for $(Sr,Ca)Pd_2As_2$ and $BaPd_2As_2$ correspondingly.

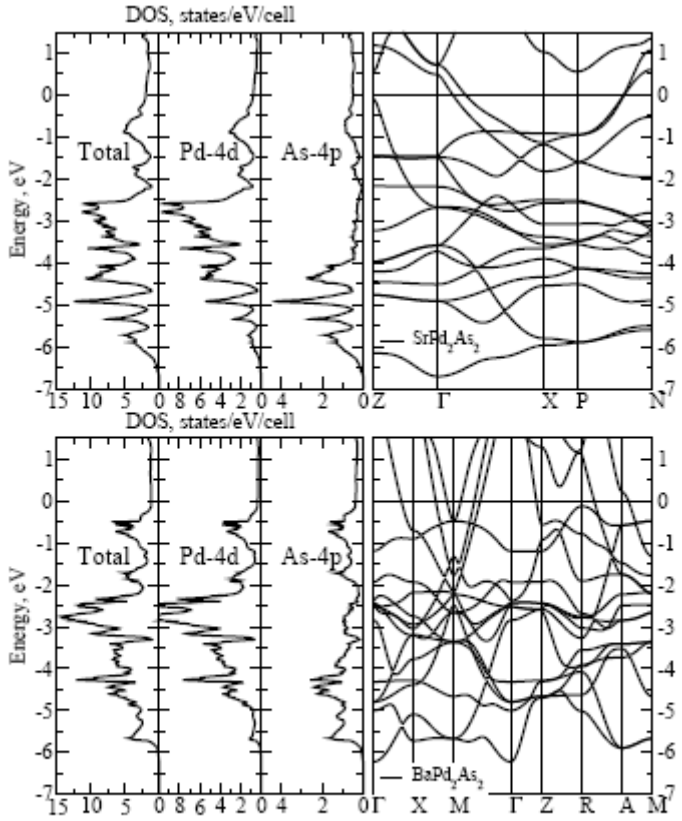


Fig. 2. LDA calculated band dispersions and densities of states of $SrPd_2As_2$ (top) and $BaPd_2As_2$ (bottom). The Fermi level is zero.

MgFeGe puzzle

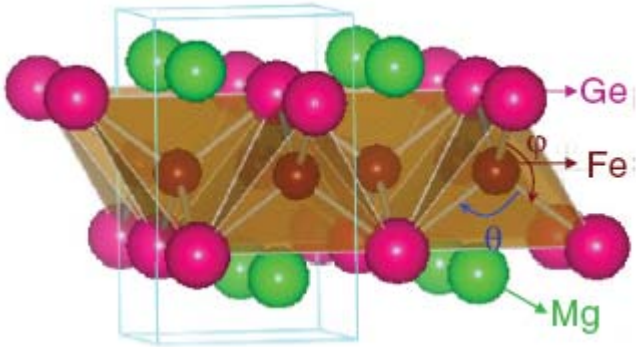
PHYSICAL REVIEW B 85, 104403 (2012)

MgFeGe as an isoelectronic and isostructural analog of the superconductor LiFeAs

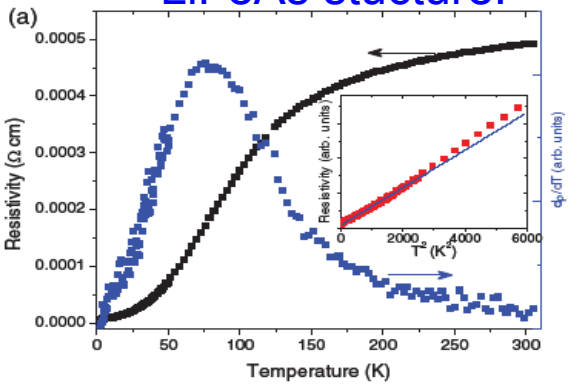
Xiaofeng Liu,[1] Satoru Matsuishi,[2] Satoru Fujitsu,[1] and Hideo Hosono[1,2,*]

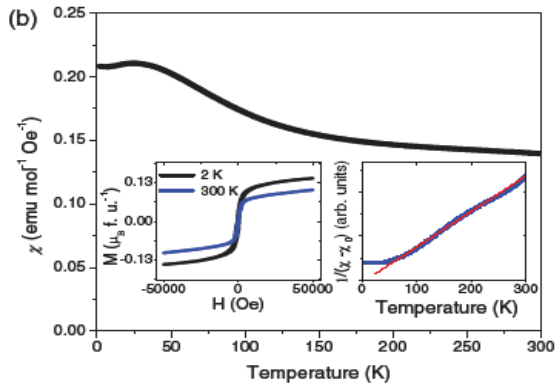
Contrast of LiFeAs with isostructural, isoelectronic, and non-superconducting MgFeGe

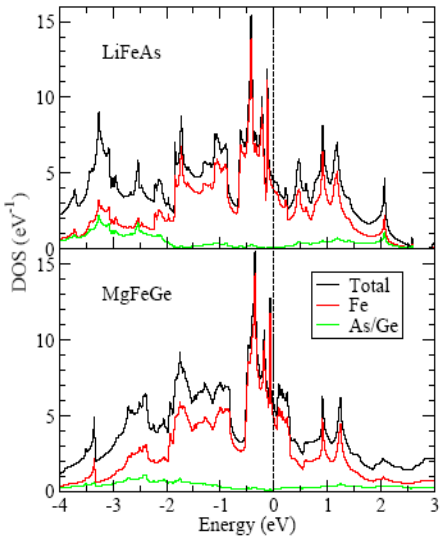
H. B. Rhee and W. E. Pickett ArXiv:1208.4180

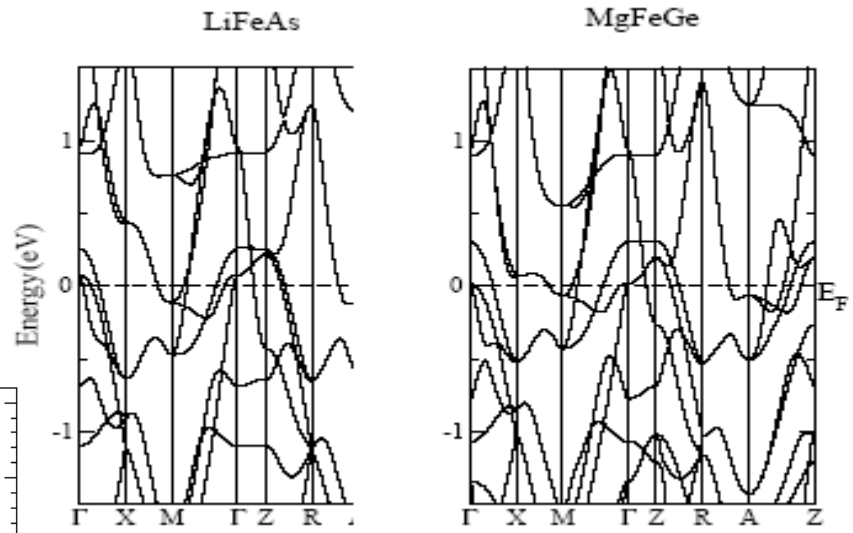


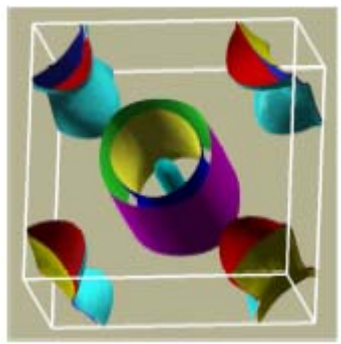
LiFeAs stucture!

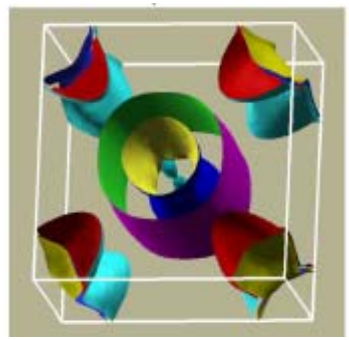












No superconductivity for T>2K!
Paramagnetic Metal!

Berndt Matthias rules:

Six rules for a successful search for new superconductors:

1 . A high symmetry is good; cubic symmetry is the best.

2. A high density of electronic states is good.

3. Stay away from oxygen.

4. Stay away from magnetism.

5. Stay away from insulators.

6. Stay away from theorists.

All these rules (with possible exception of #6) have been proven wrong in cuprates!

“Iron Age” rules (due to Mazin):

Present day theoretical advices:

1 . A high symmetry is good; cubic symmetry is the best.

New rule: ***Layered structures are good***

2. A high density of electronic states is good.

New rule: ***Carrier density should not be too high***

3. Stay away from oxygen.

New rule: ***3d metals (V, Cr, Mn, Fe, Co, Ni, Cu) are good***

4. Stay away from magnetism.

New rule: ***Antiferromagnetism is essential***

5. Stay away from insulators.

New rule: ***Fermi surface geometry is essential (to match with spin excitations?)***

6. Stay away from theorists.

New rule: ***Enlist theorists, at least to compute the Fermi surfaces!***

What (if any) electronic structure (Fermi Surface) is helpful for high Tc?

1. Low dimensionality?
2. Multiple bands?
3. High values of DOS at the Fermi level?
4. Nesting? Apparently Not !
5. And what about MgFeSe?!

Conclusions

- Total DOS at the Fermi level directly correlates with T_c, but details depend on partial DOS'es
- AFe_2Se_2 electronic spectrum is significantly different from that of FeAs systems and pure FeSe
- No Nesting in AFe_2Se_2 !
- AFe_2Se_2 – more correlated!
- Single layer FeSe – T_c ~ 50K!
- New Pt,Pd – pnictide superconductors – multiple band, but low T_c!
- Is where any "optimal electronic structure"?