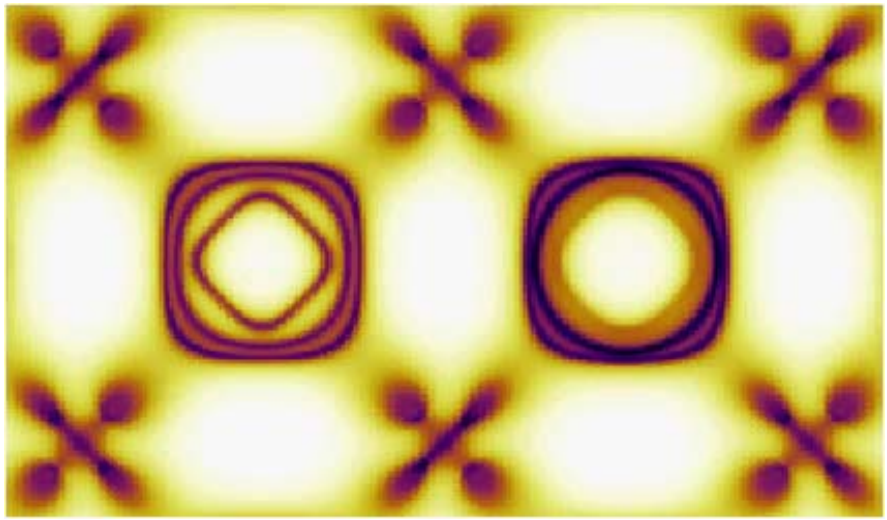
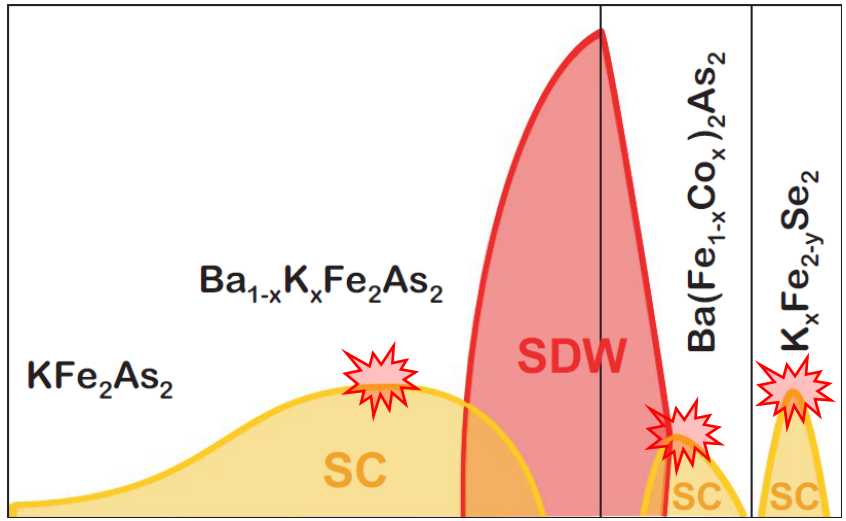
Complex electronic structure of iron-based superconductors as a key to high temperature superconductivity





Alexander Kordyuk

Institute of Metal Physics, Kiev, Ukraine

What can we learn from ARPES?

- **Electronic structure =**
  electronic band structure +
  structure of interaction (self-energy)
- **ARPES on HTCS: self-energy**
- **ARPES on FeCS: band structure**

What can we learn from ARPES?

- **Electronic structure =**
  electronic band structure +
  structure of interaction (self-energy)

Electronic band structure defines electro-magnetic properties of metals
(inc. “strongly correlated”)

"entities should not be multiplied beyond necessity"

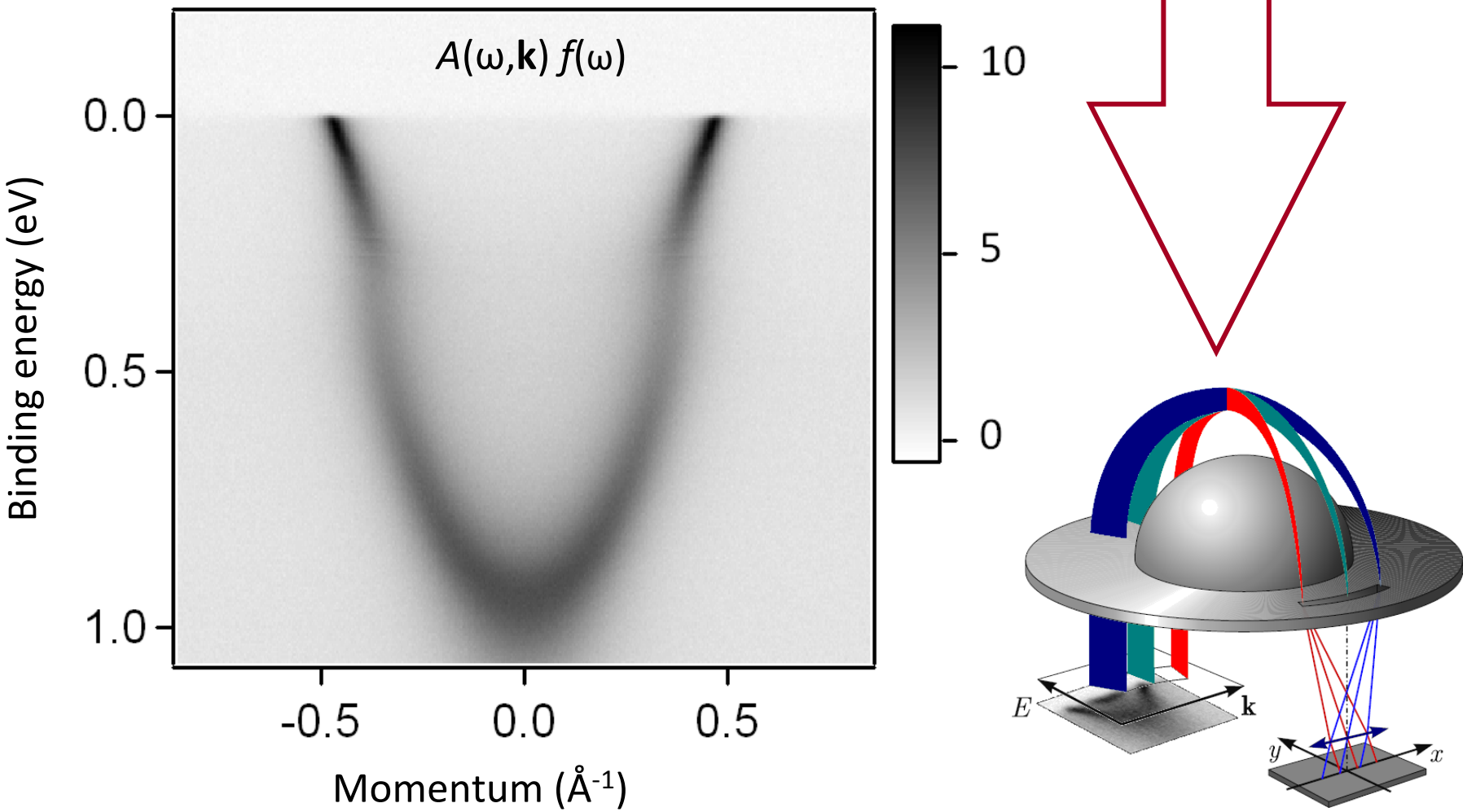
Occam's razor

What can we learn from ARPES?

- **Electronic structure =**
  electronic band structure +
  structure of interaction (self-energy)
- **ARPES on HTCS: self-energy**
- **ARPES on FeCS: band structure**

Electronic structure

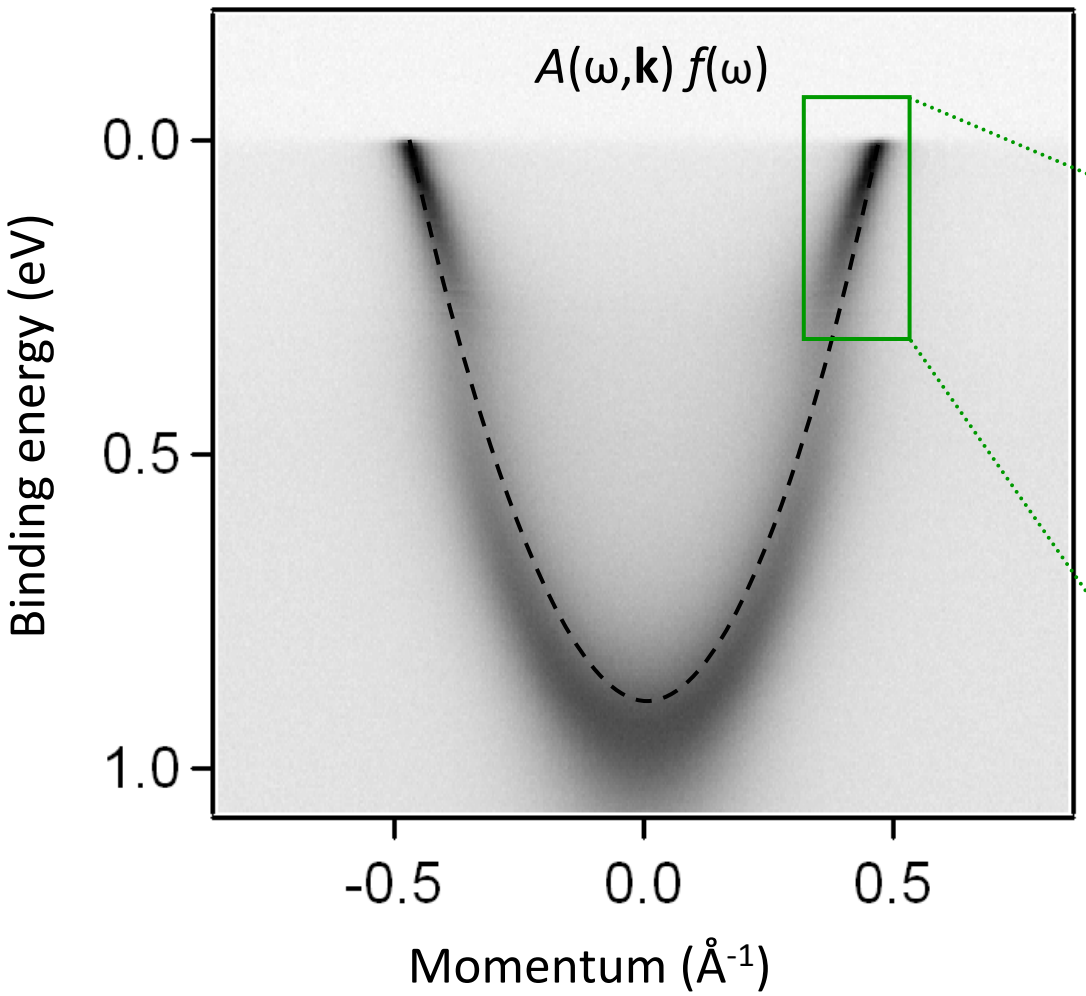
Electronic spectrum ≡ Spectrum of one-electron excitations ≡ Probability to find electron with momentum **k** and energy ω



Structure of electronic spectrum

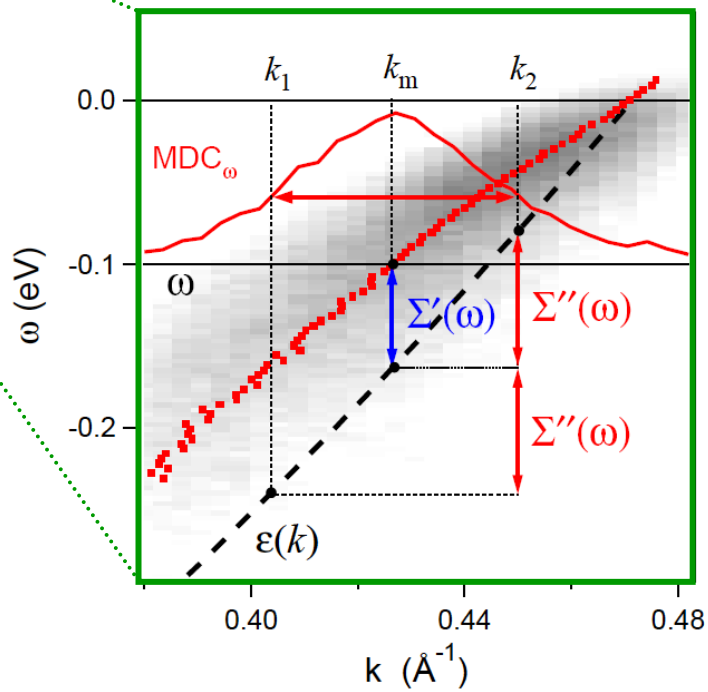
Spectral function

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(\mathbf{k}) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$



ε(k) – "bare" electronic band structure

Σ(ω,k) – self-energy

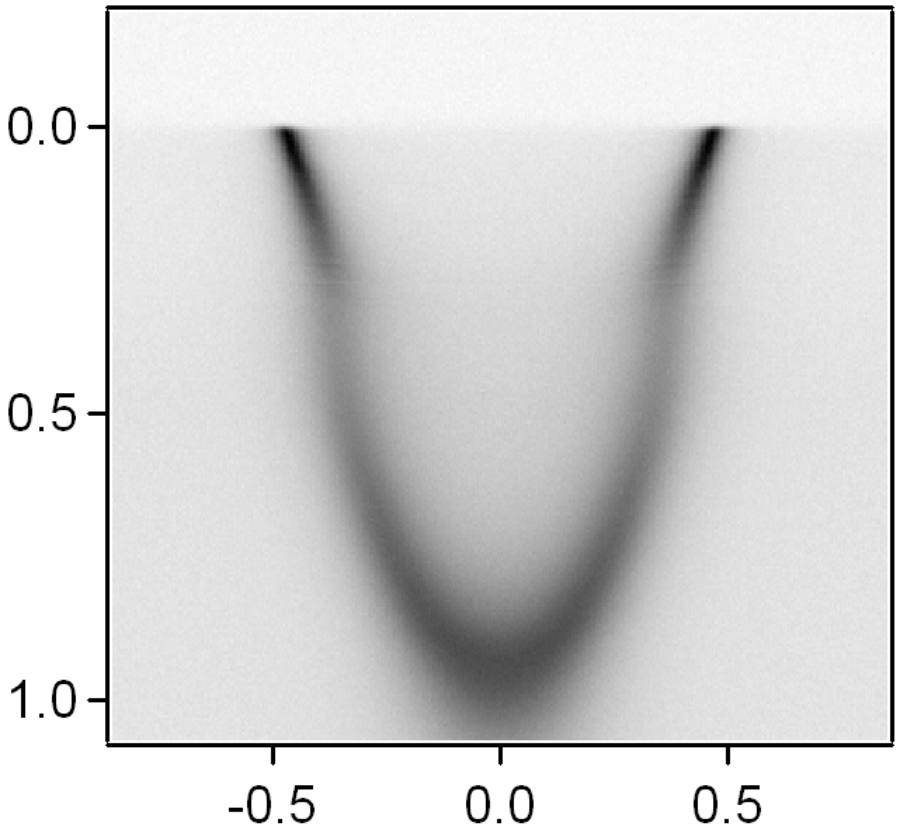


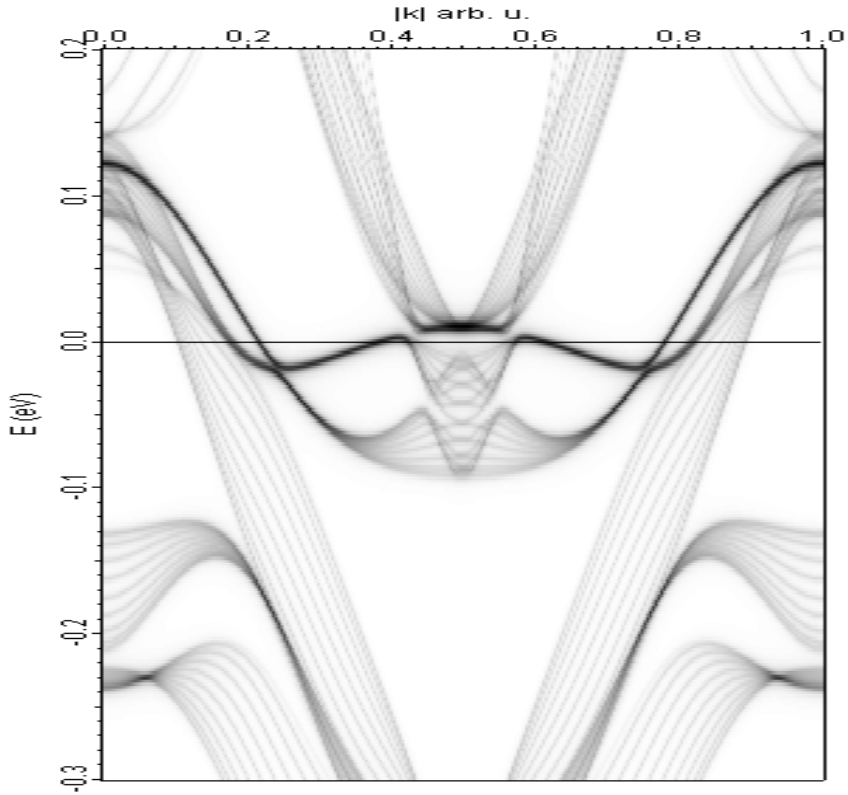
Kordyuk *PRB* 2005

Electronic spectrum =

band structure + self-energy

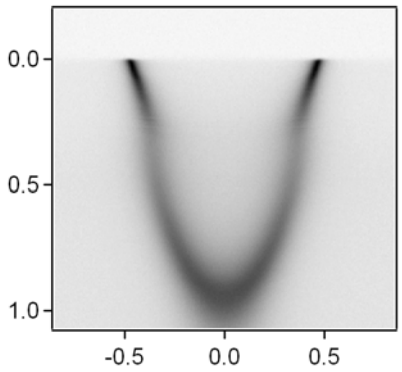
Cu-SC *vs* Fe-SC

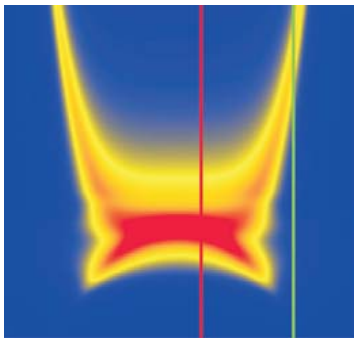




Cu-SC *vs* Fe-SC

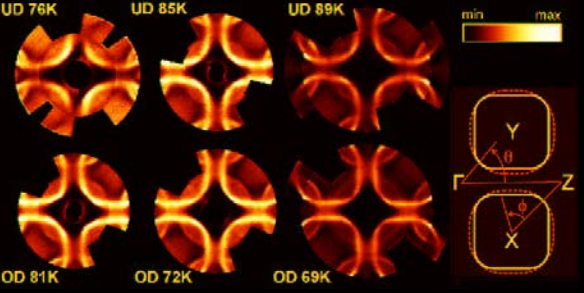
Cuprates

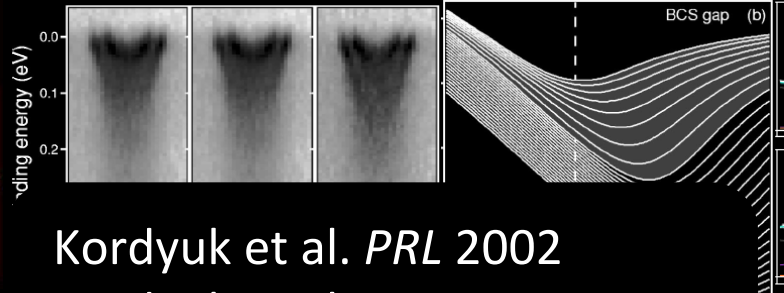


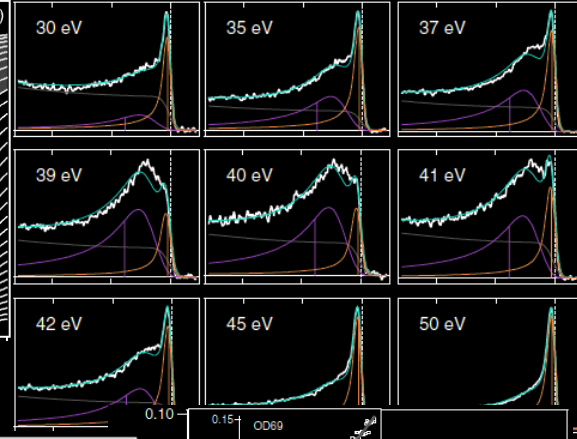


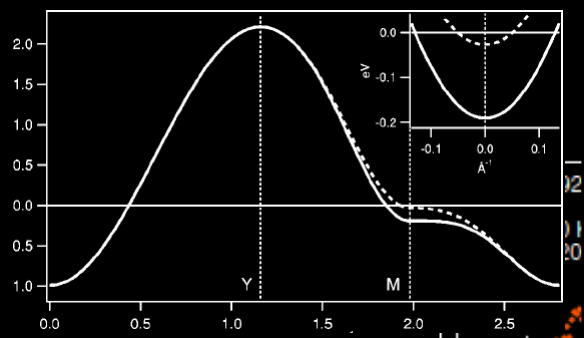
Band structure is simple but...

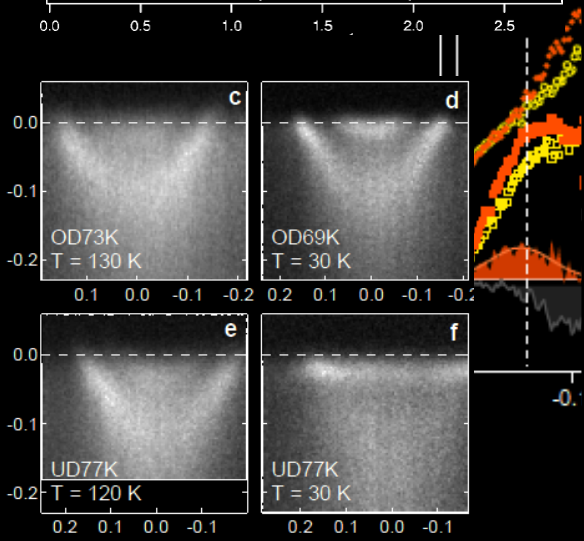
complexity of the **cuprates** is encapsulated in complex **kω-dependence of the self-energy** that is defined by the spectrum of **spin-fluctuations**

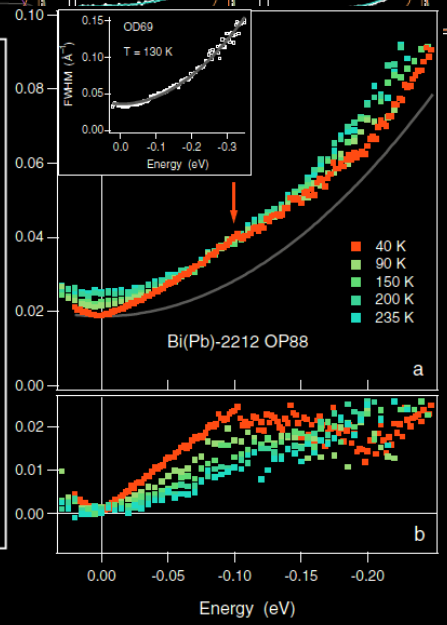


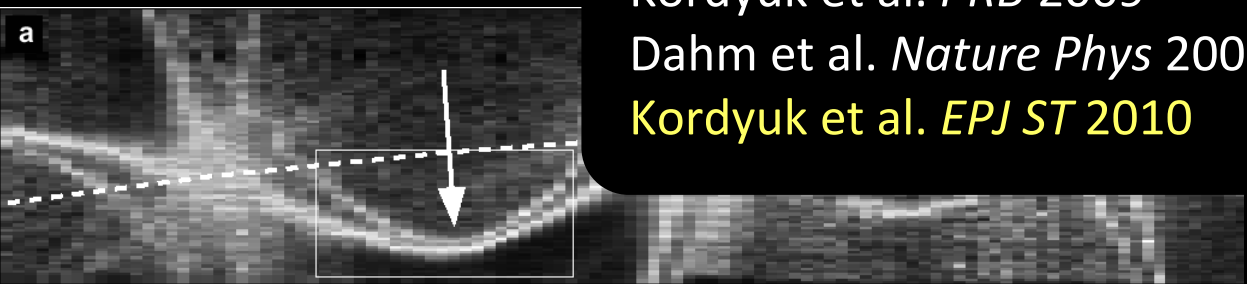


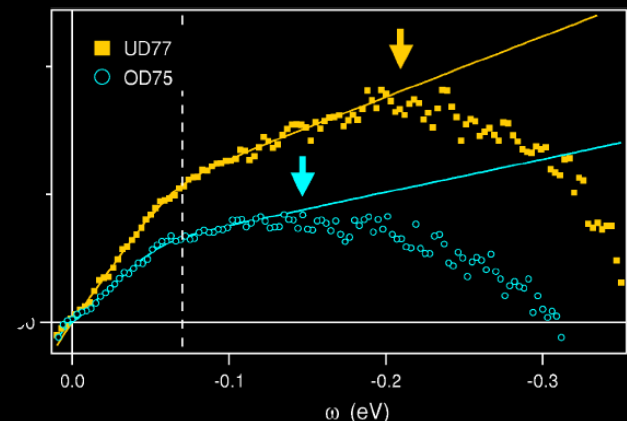








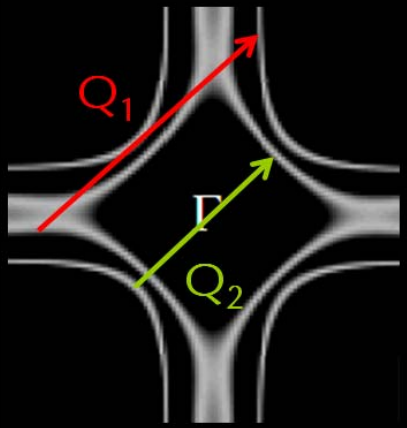




Kordyuk et al. *PRL* 2002
Kordyuk et al. *PRB* 2002
Borisenko et al. *PRL* 2003
Kim et al. *PRL* 2003
Kordyuk et al. *PRL* 2004
Kordyuk et al. *PRB* 2004
Borisenko et al. *Nature* 2004
Borisenko et al. *PRL* 2004
Kordyuk et al. *PRB* 2005
Kordyuk et al. *PRL* 2006
Borisenko et al. *PRL* 2006
Kordyuk & Borisenko *FNT* 2006
Inosov et al. *PRL* 2007
Inosov et al. *PRB* 2008
Kordyuk et al. *PRB* 2009
Dahm et al. *Nature Phys* 2009
Kordyuk et al. *EPJ ST* 2010

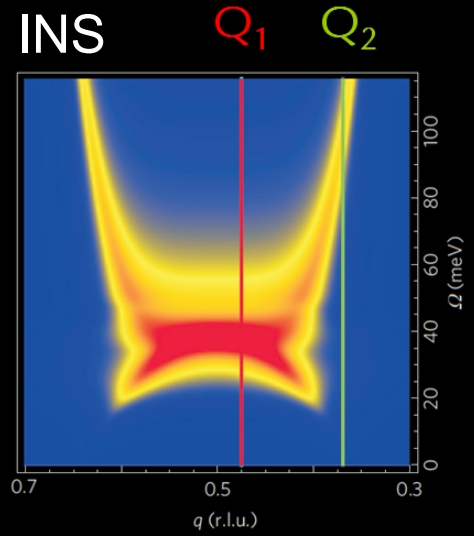
Spin-fluctuations and superconductivity

ARPES

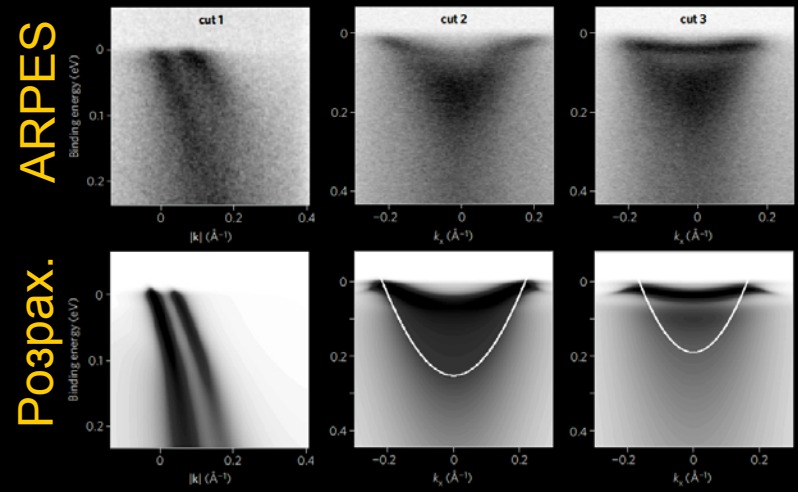


Im $G_0(\mathbf{k},\omega)$

INS



Im $\chi(\mathbf{q},\Omega)$



Im $G(\mathbf{k},\omega)$

Formula of cuprates:

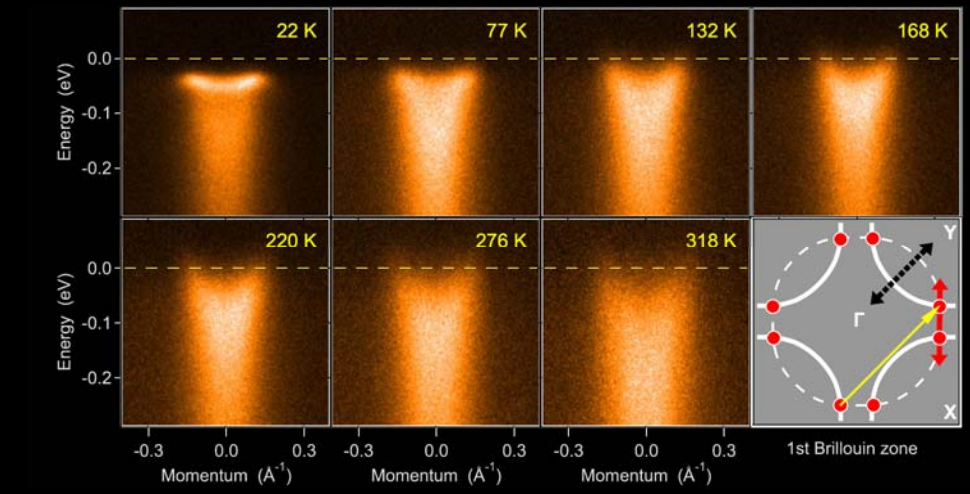
$$G_0^{-1} + \overbrace{\alpha^2 G \star \chi}^{\Sigma} = G^{-1}$$

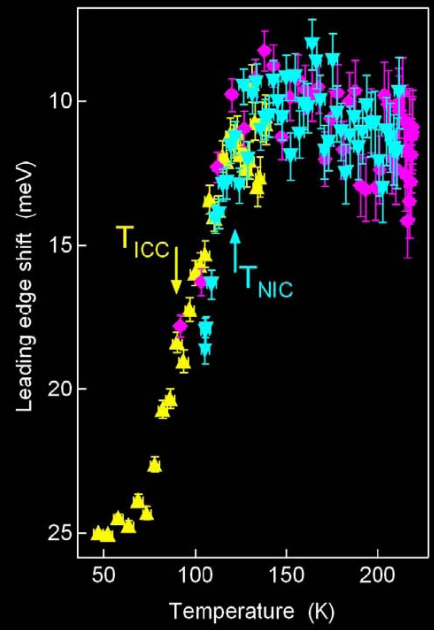
$$G_0^{-1} + \alpha^2 G \star \overbrace{G \star G}^{\chi} = G^{-1}$$

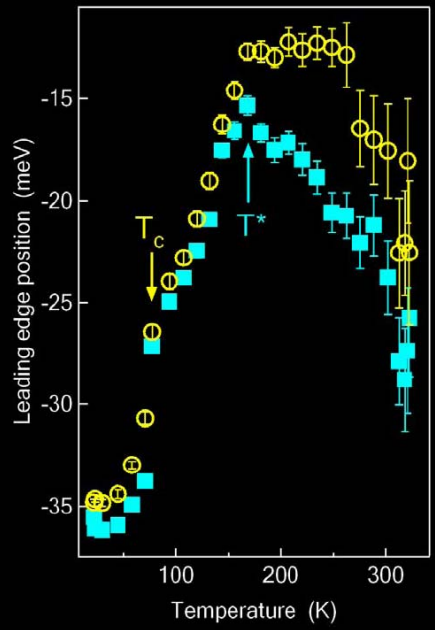
1. ARPES and INS
   -> spin-fluctuations
2. T_c ~ 150 K.

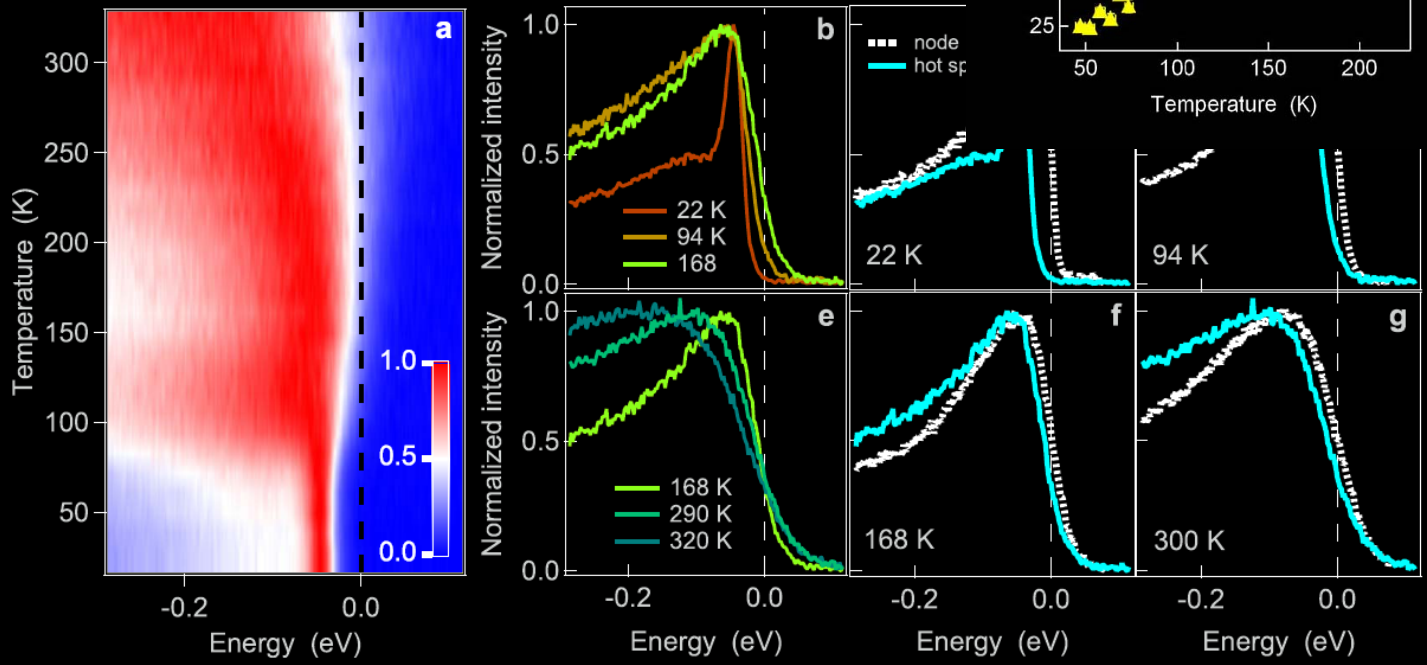
D. Inosov et al., *PRB* 2007
T. Dahm et al., *Nature Phys* 2009
A. Kordyuk et al., *EPJ ST* 2010

Non-monotonic pseudogap in BSCCO



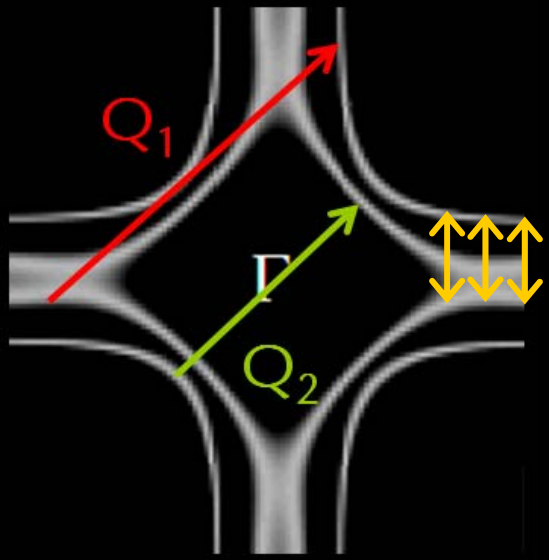






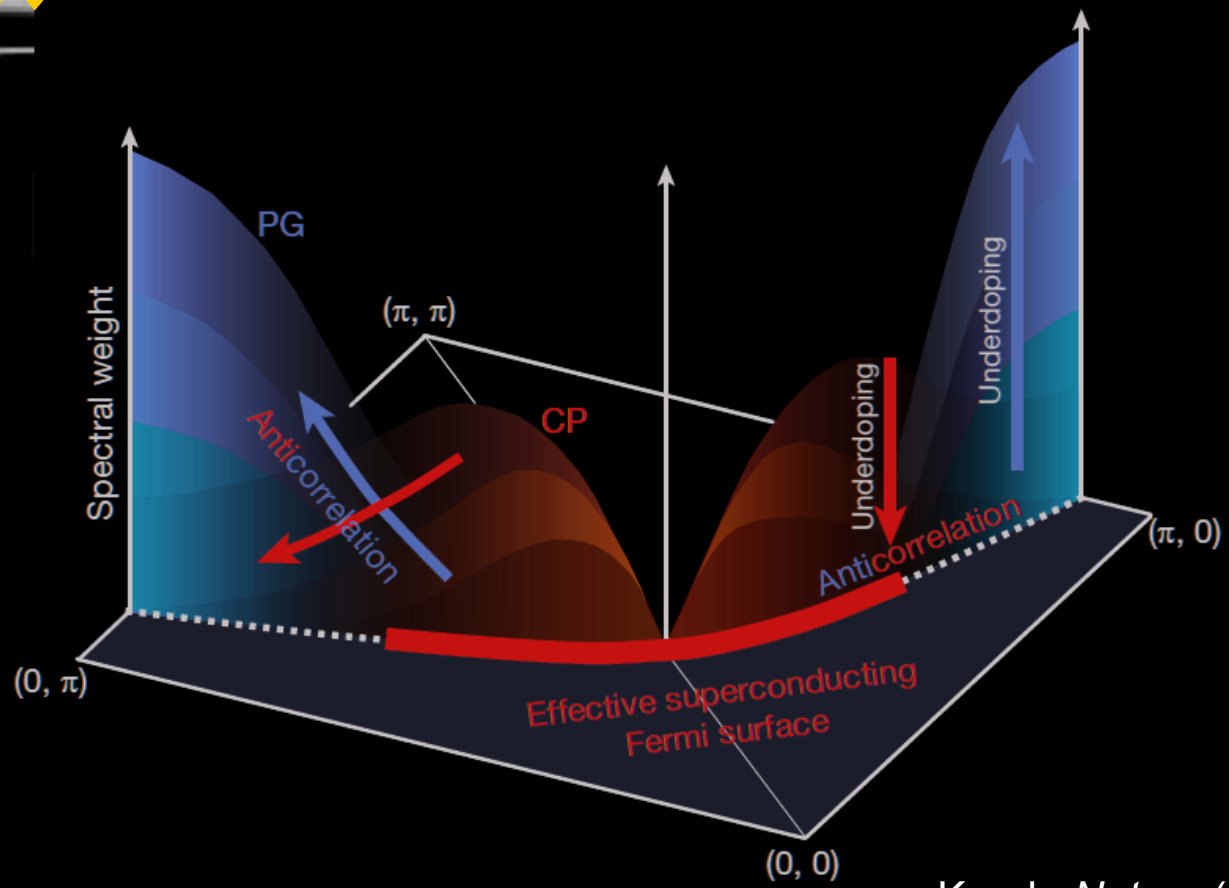
Kordyuk *PRB* (2009)

“Two-gap scenario"



SDW and superconductivity compete for the phase spase

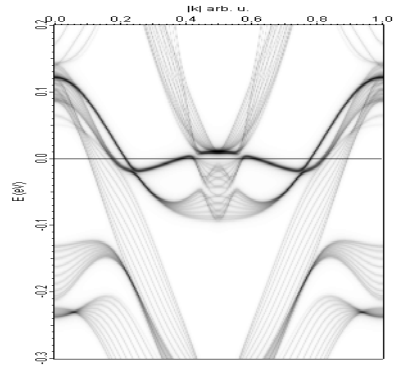
“FS nesting”



Kondo *Nature* (2009)

Cu-SC *vs* Fe-SC

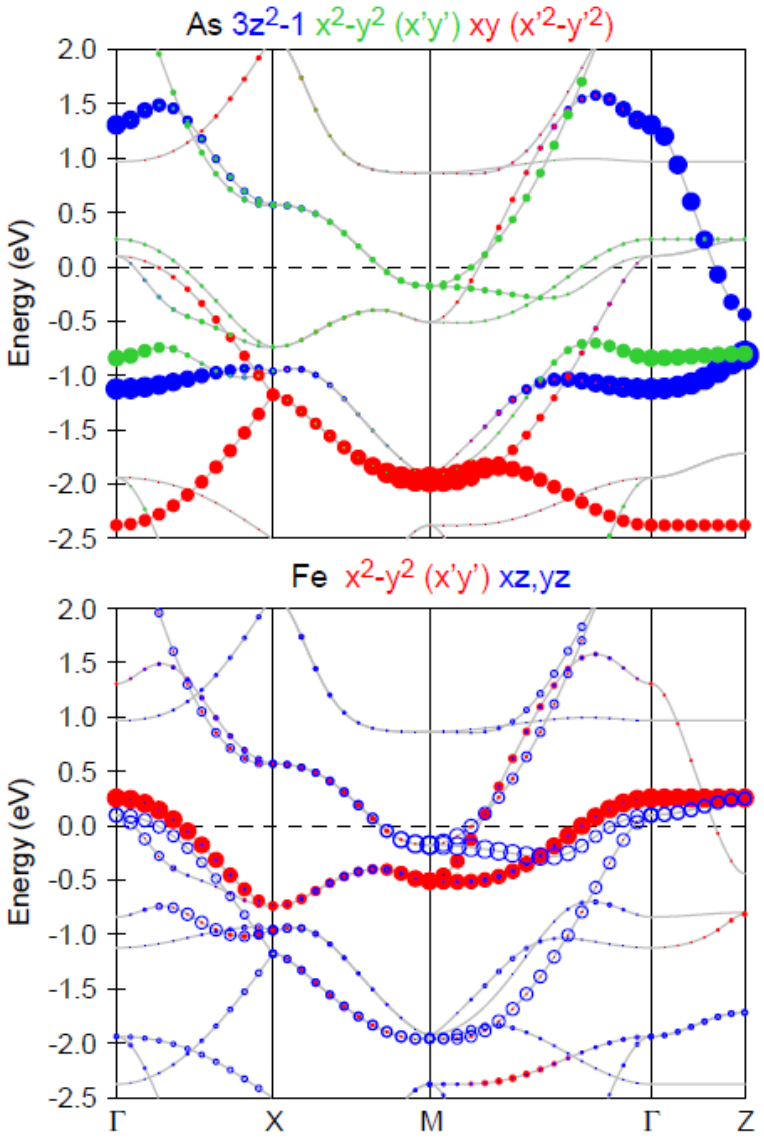
Fe-SC

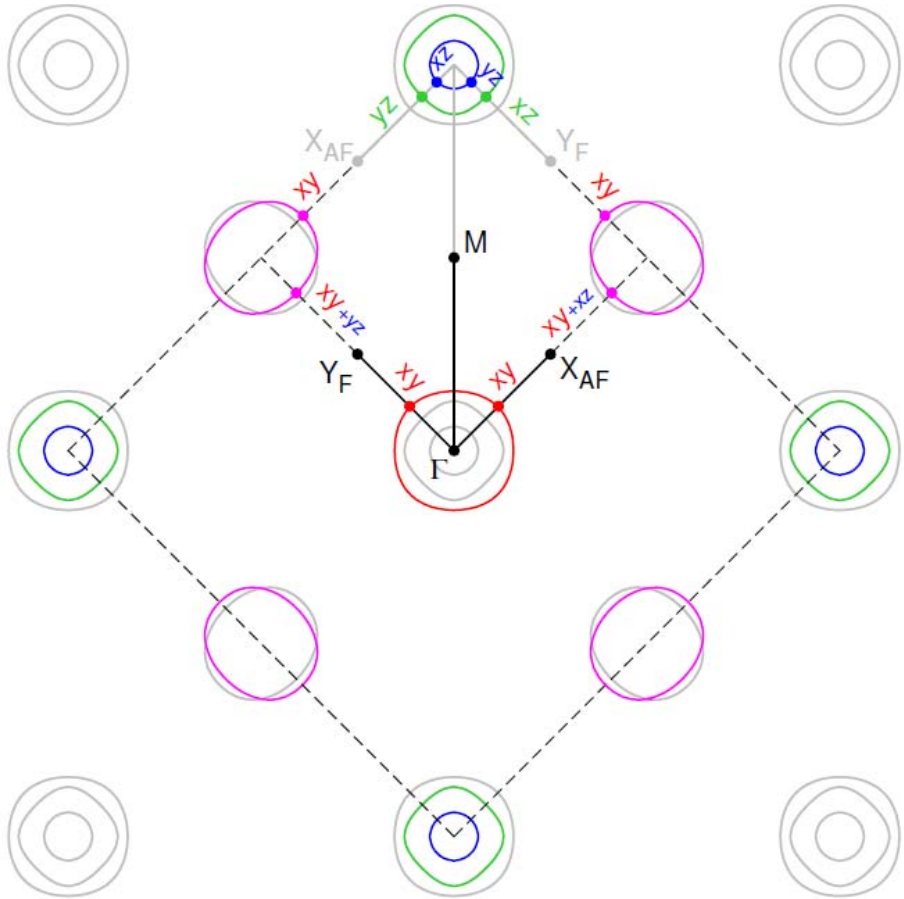


Complexity of **Fe-SC** is in **complex band structure**. Both phonons and SFs are importand but multi-band effects should be taken into account

ARPES + LDA + self-energy analysis

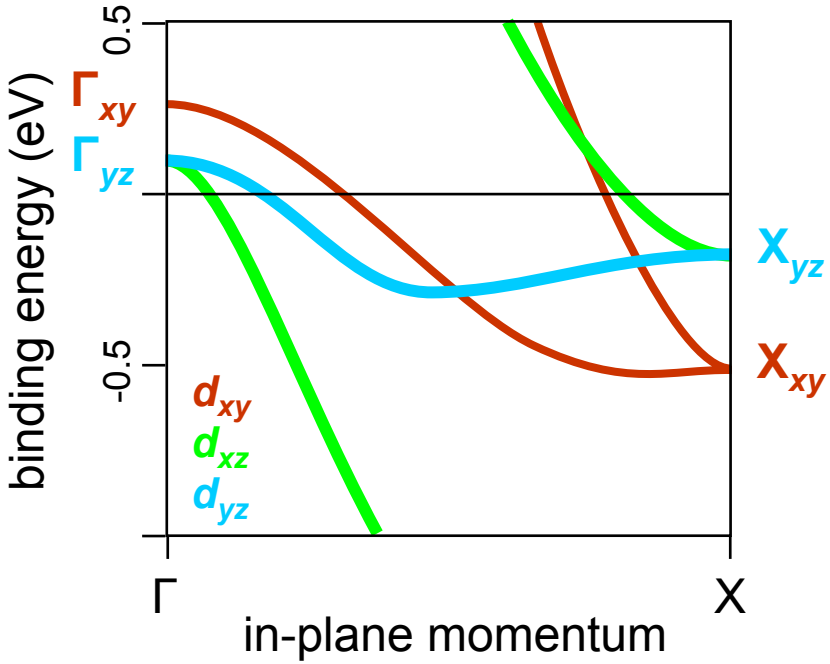
FeSC electronic band structure

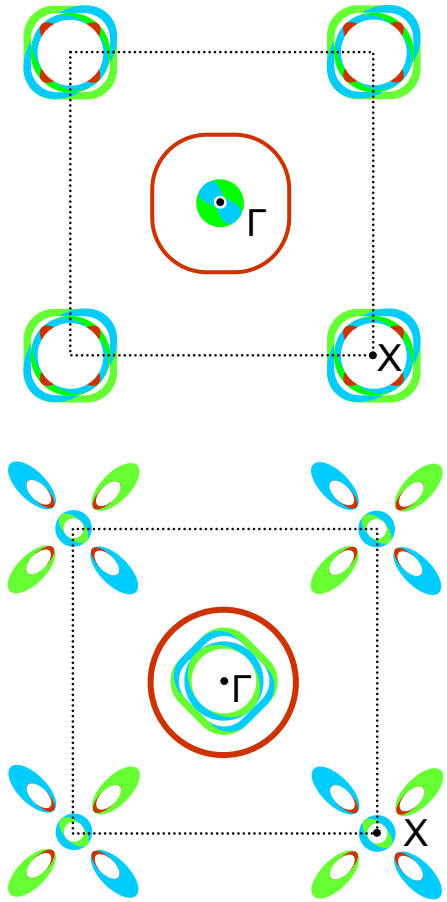


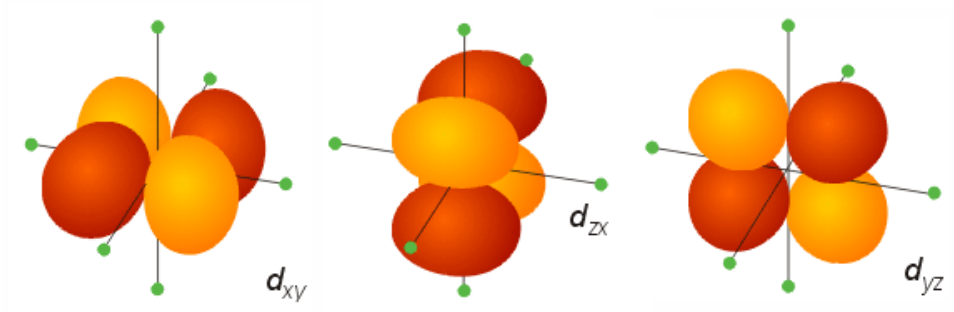


Yaresko 2010

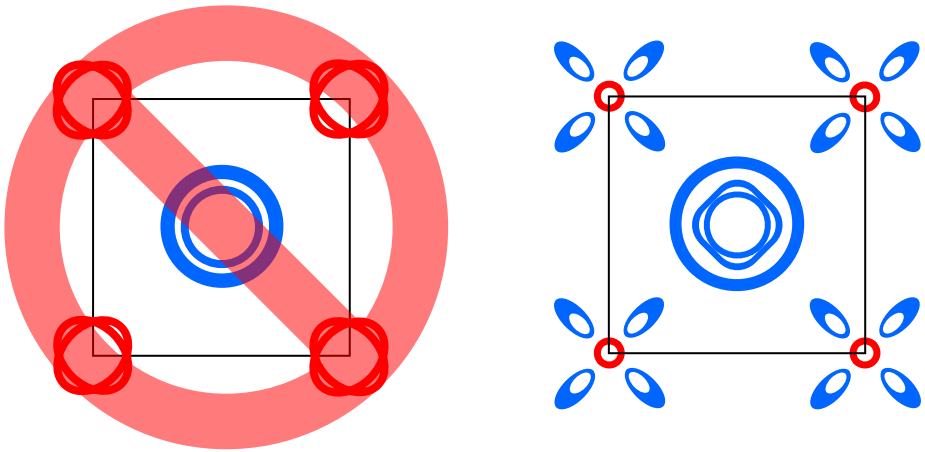
Iron-based superconductors: electronic structure

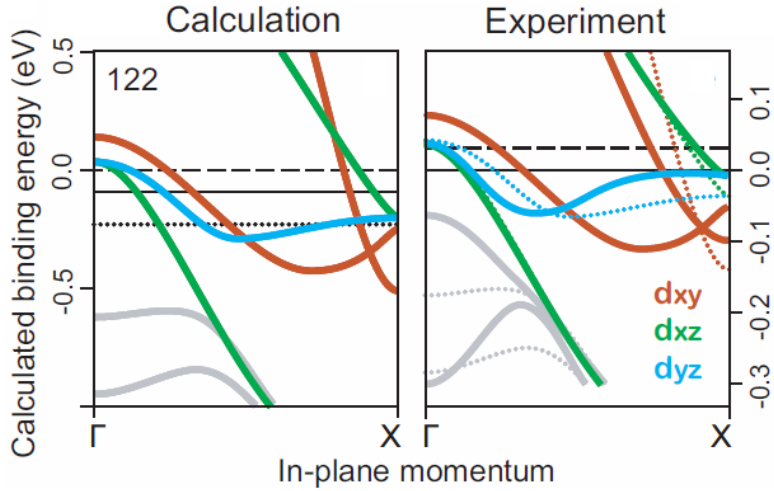




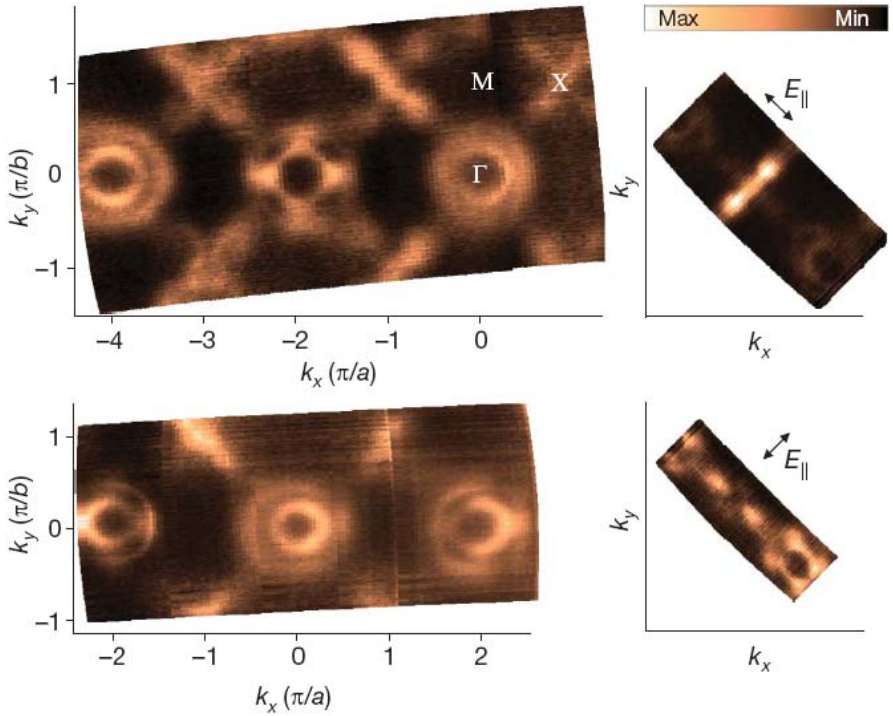


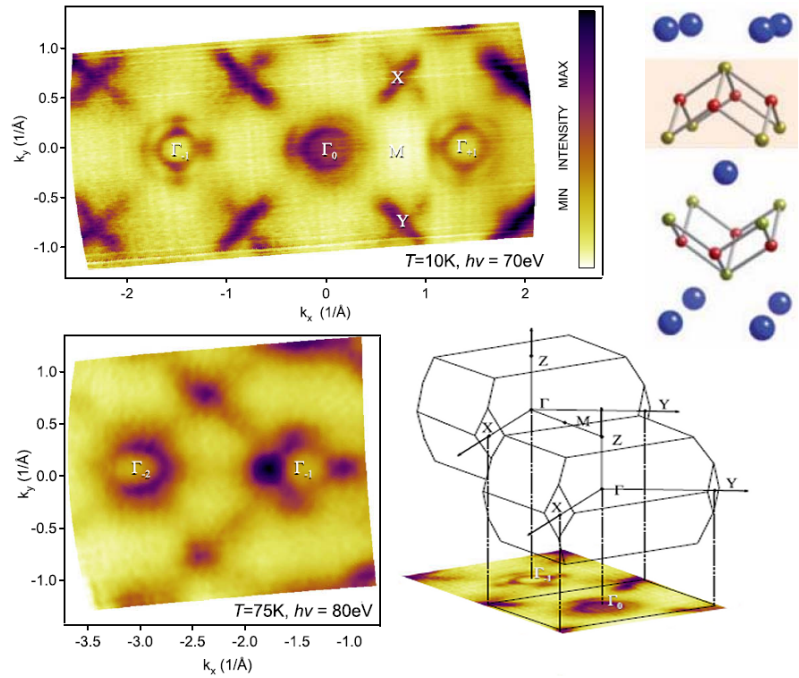
Fermi surface of BKFA





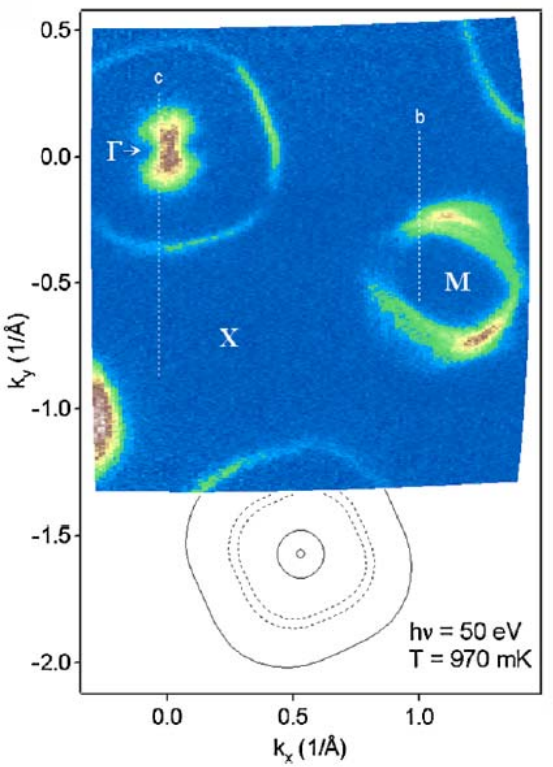
A. A. Kordyuk, *J. Supercond. Nov. Magn.* 2013

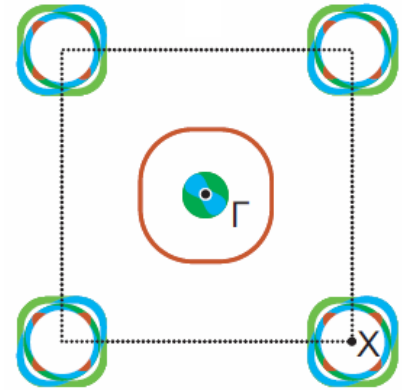


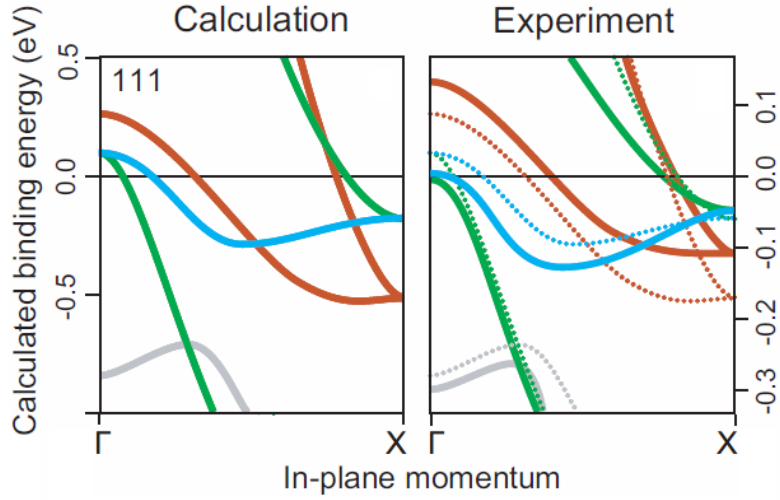


V. Zabolotnyy *Nature* 2009

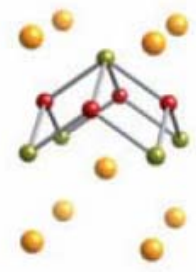
Fermi surface of LiFeAs

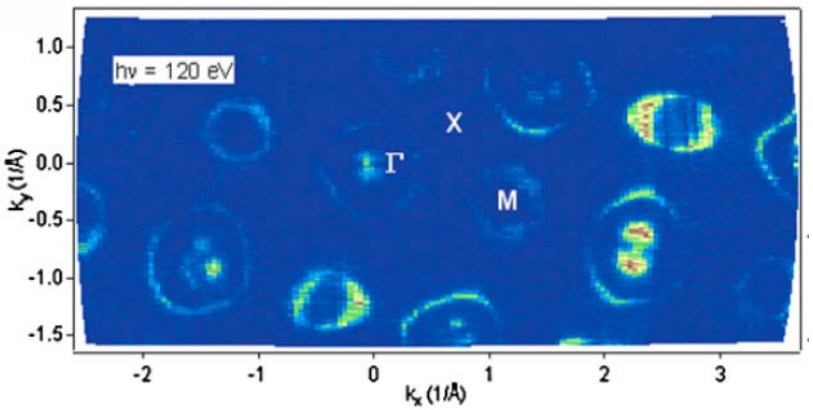






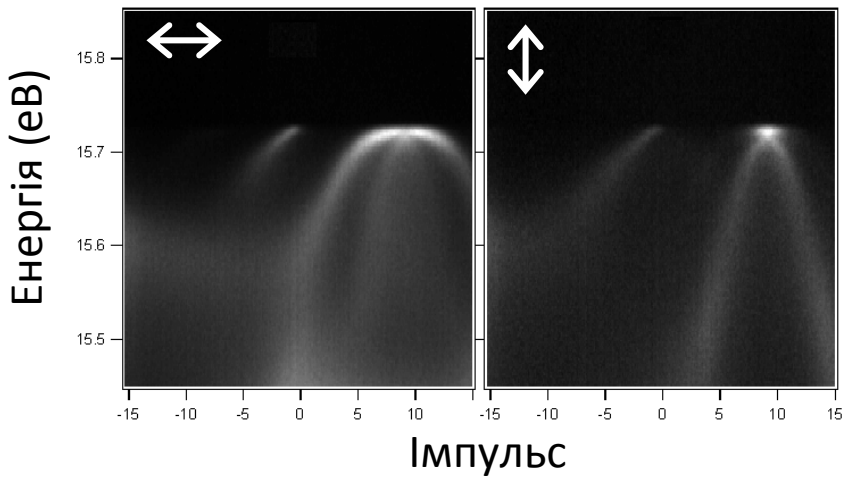
Kordyuk, *J. Supercond. Nov. Magn.* 2013





Borisenko *PRL* 2010

polarization



Kordyuk *PRB* 2010

Small Fermi surfaces

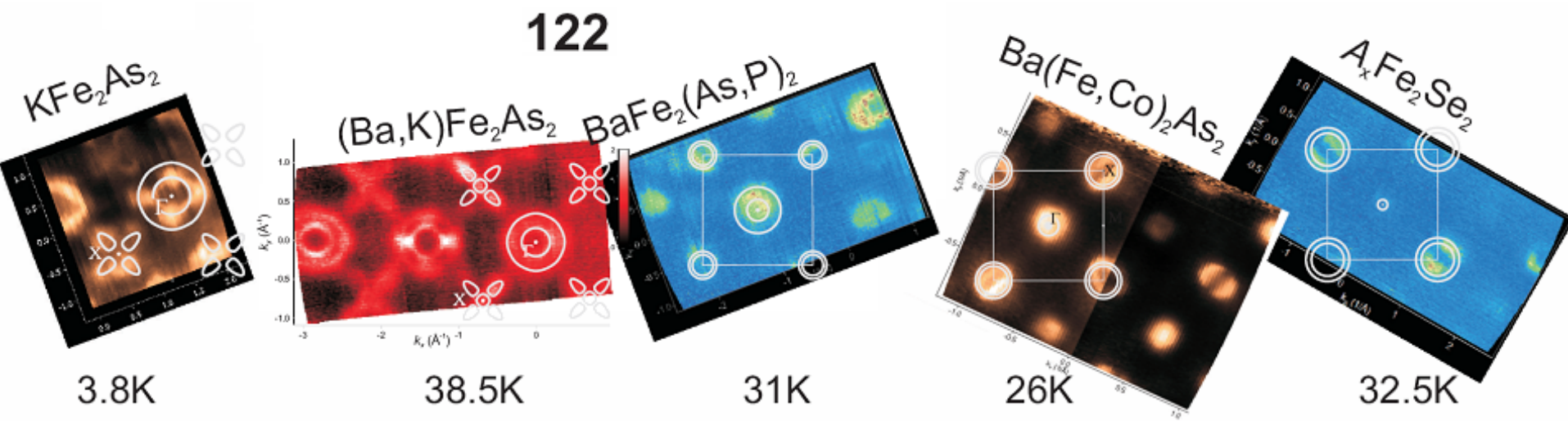
=

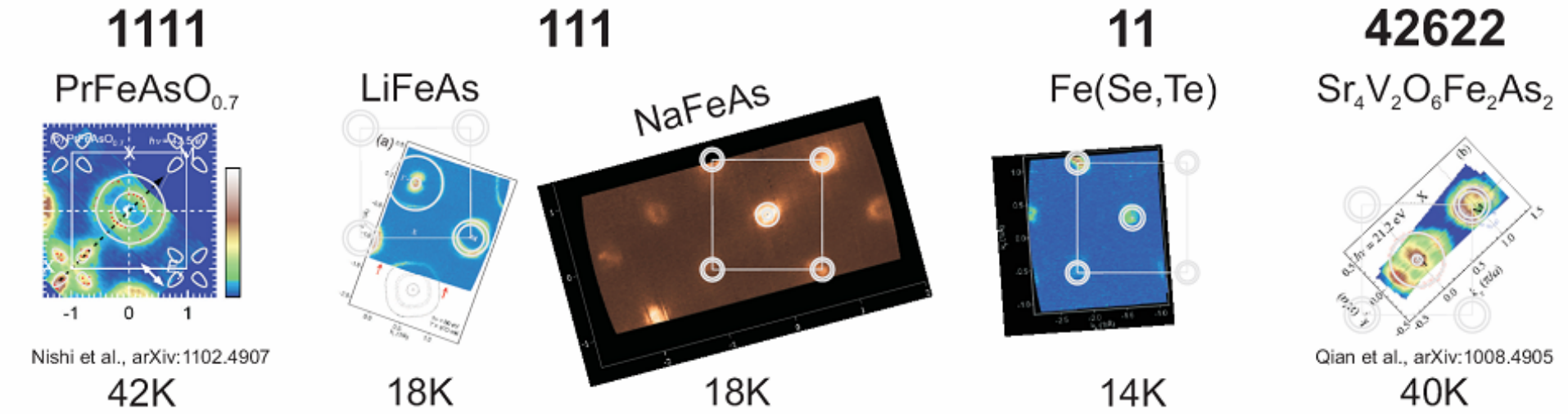
vicinity to Lifshitz transition

=

vicinity to 2D-3D crossover

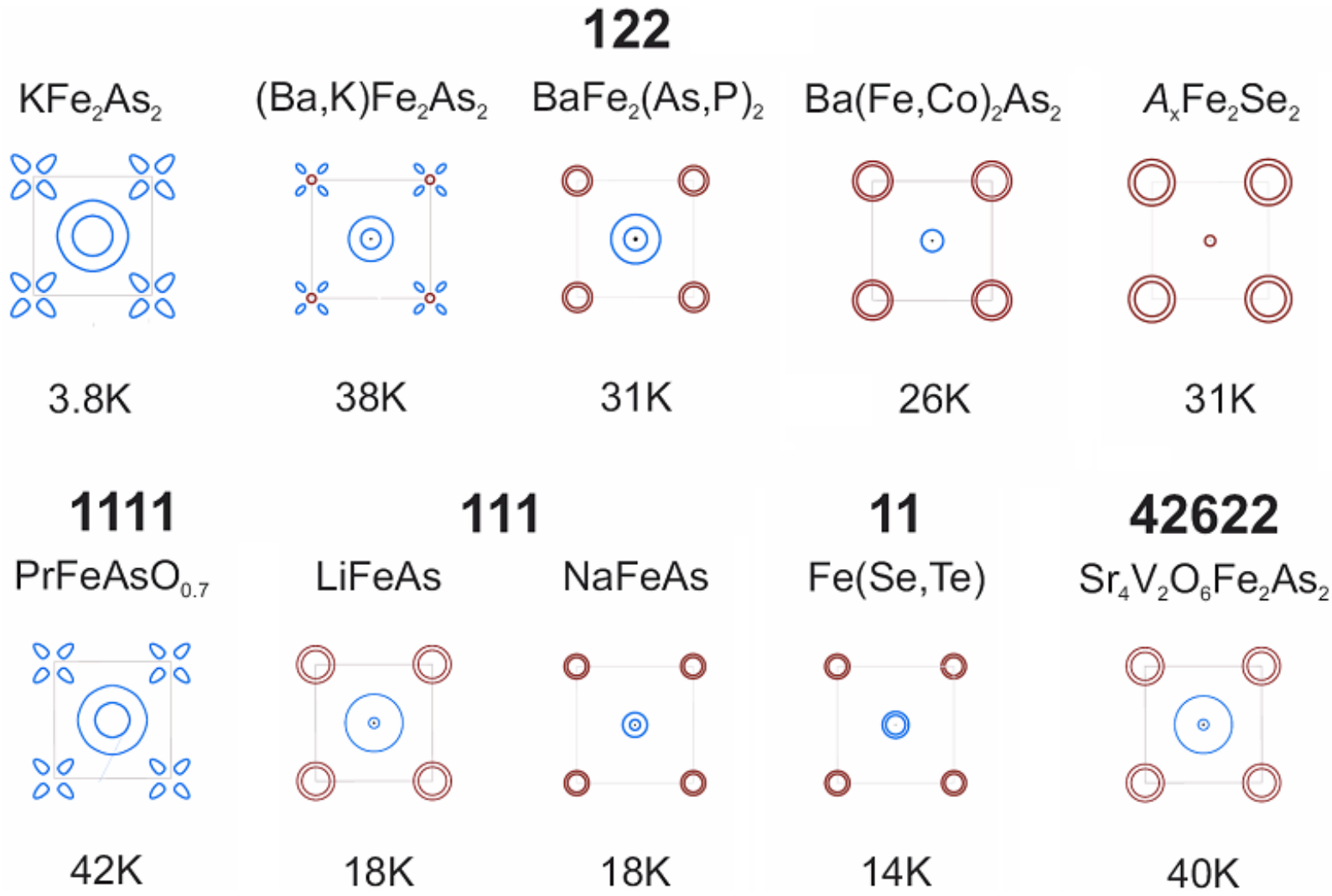
FS‘s of iron-based superconductors





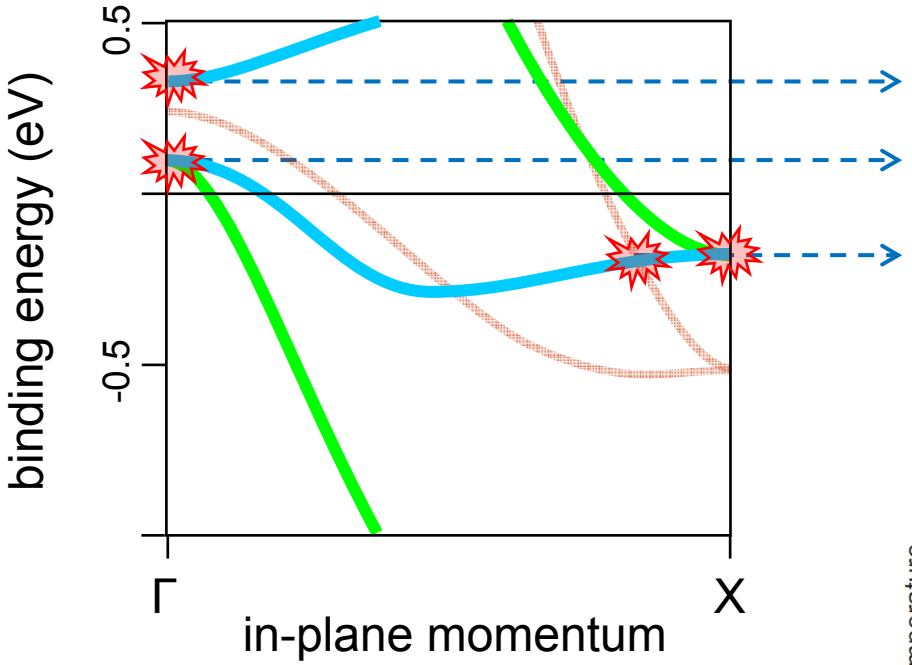
D. Evtushinsky 2011

FS‘s of iron-based superconductors



D. Evtushinsky 2011

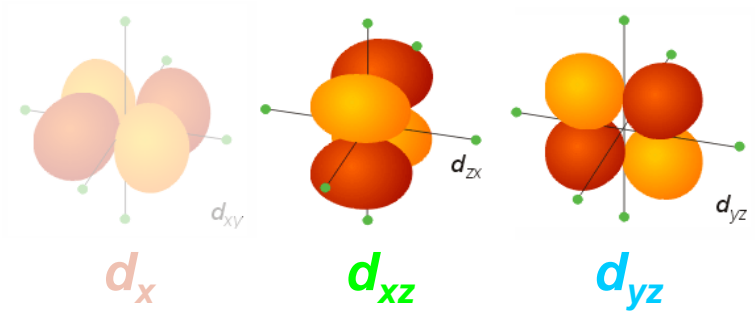
FeSC: electronic structure and superconductivity



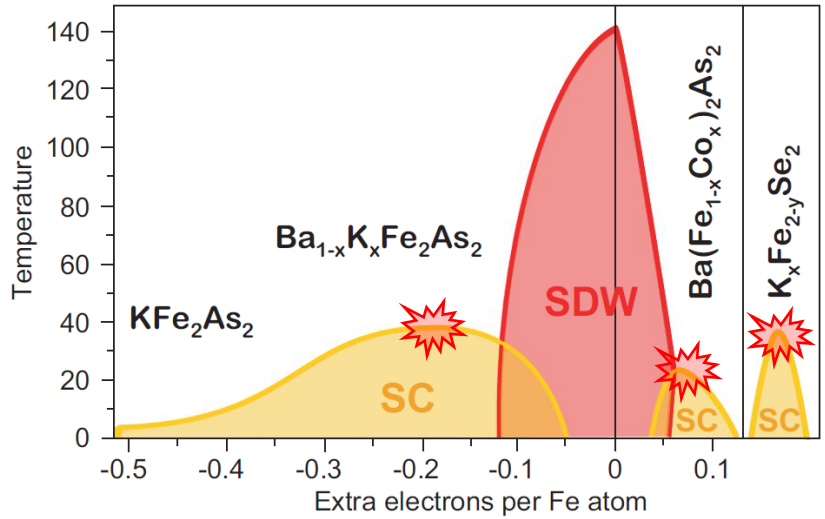
$A_xFe_2Se_2$ (31K)

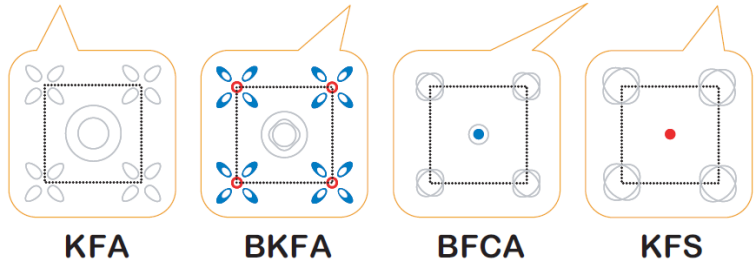
BFCA (26K)
LiFeAs (18K)

BKFA (38K)



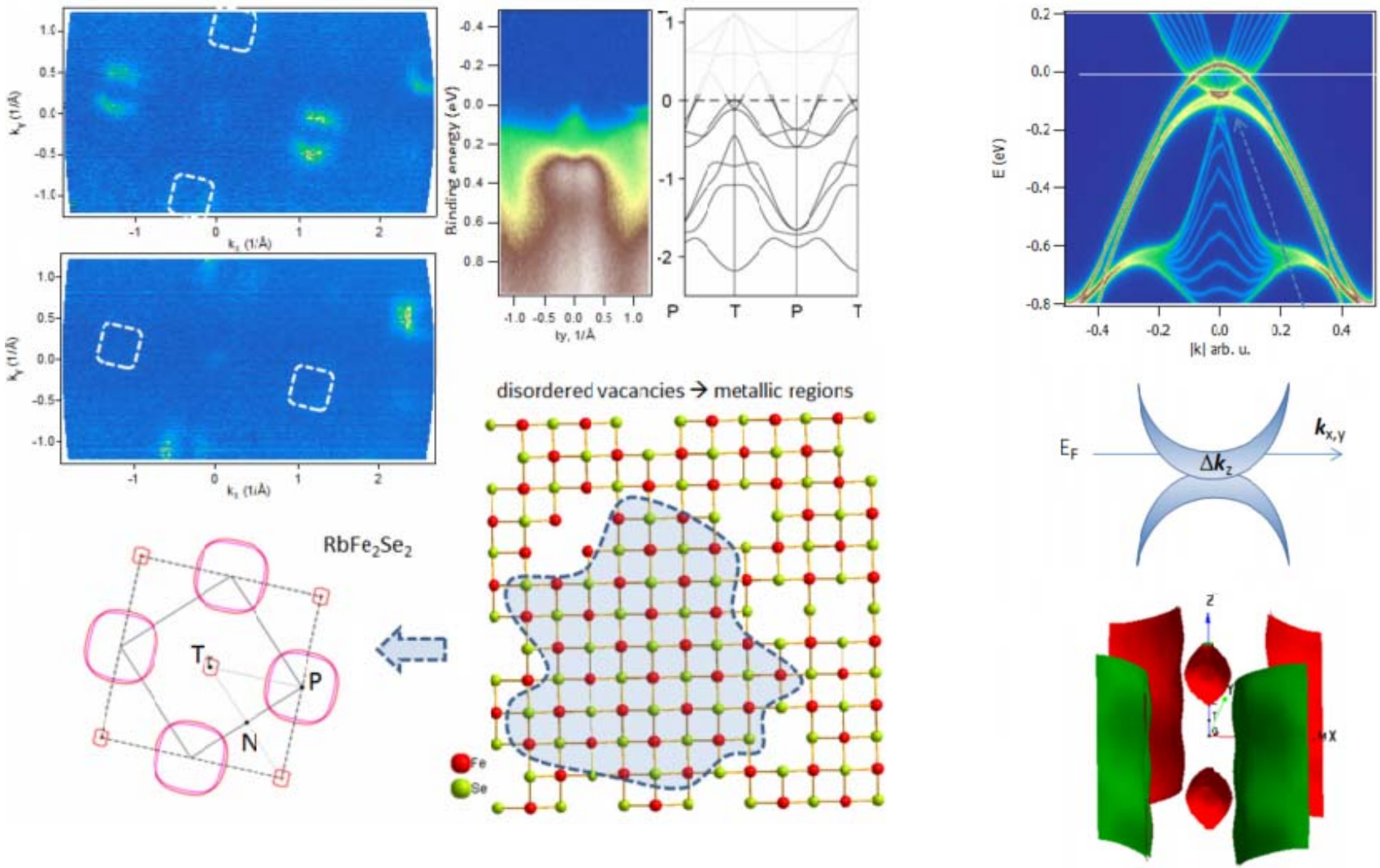
correlates with SC gap!!! - Daniil





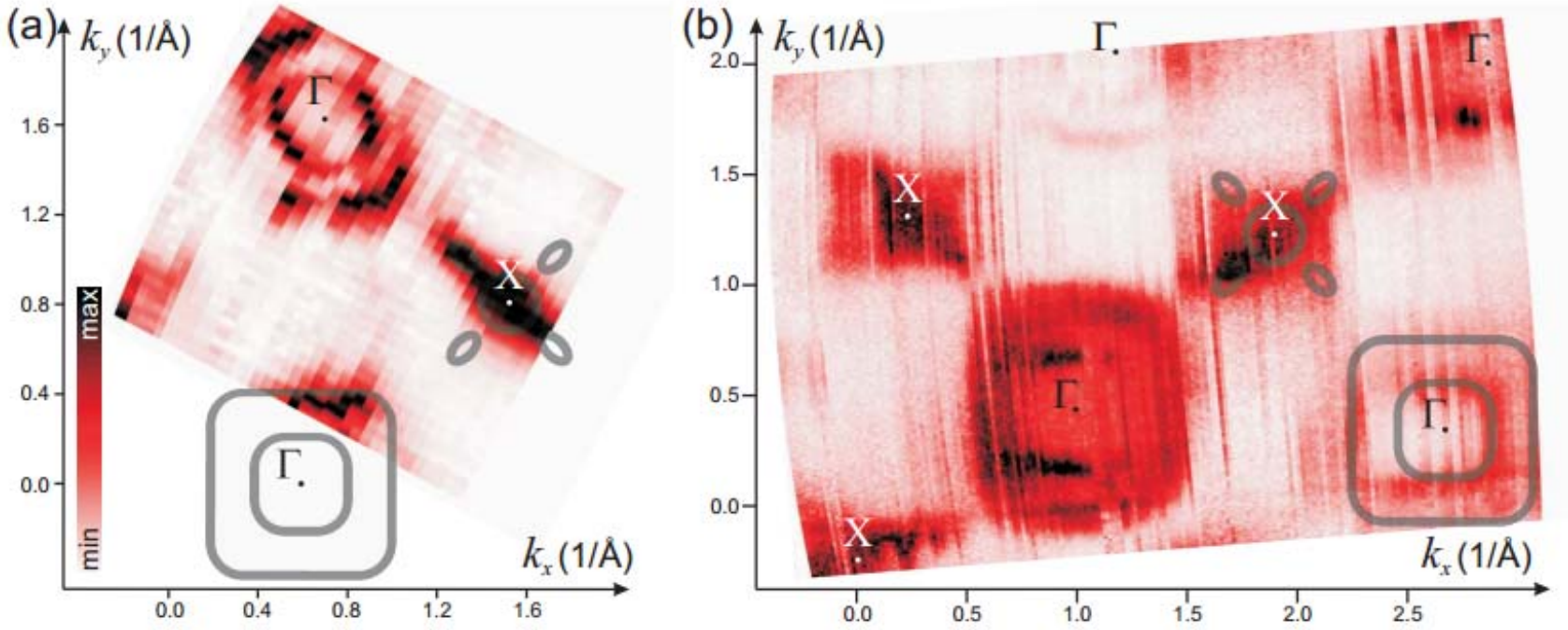
A. A. Kordyuk, *J. Supercond. Nov. Magn.* (2013)
A. A. Kordyuk et al., *Phys. Rev. B* **83**, 134513 (2011)

A-FeSe $Rb_{0.77}Fe_{1.61}Se_2$ T_c = 32.6 K



S. V. Borisenko arXiv:1204.1316 – PRB 2013

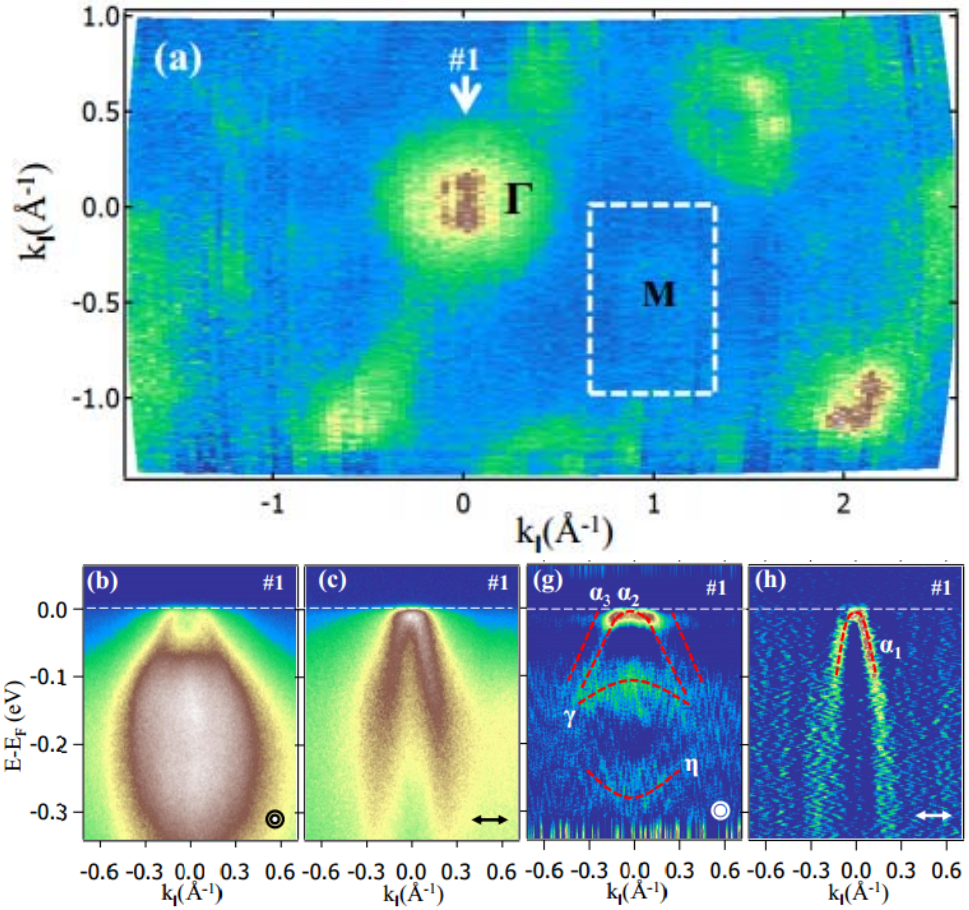
$Ca_{1-x}Na_xFe_2As_2$ **33K**

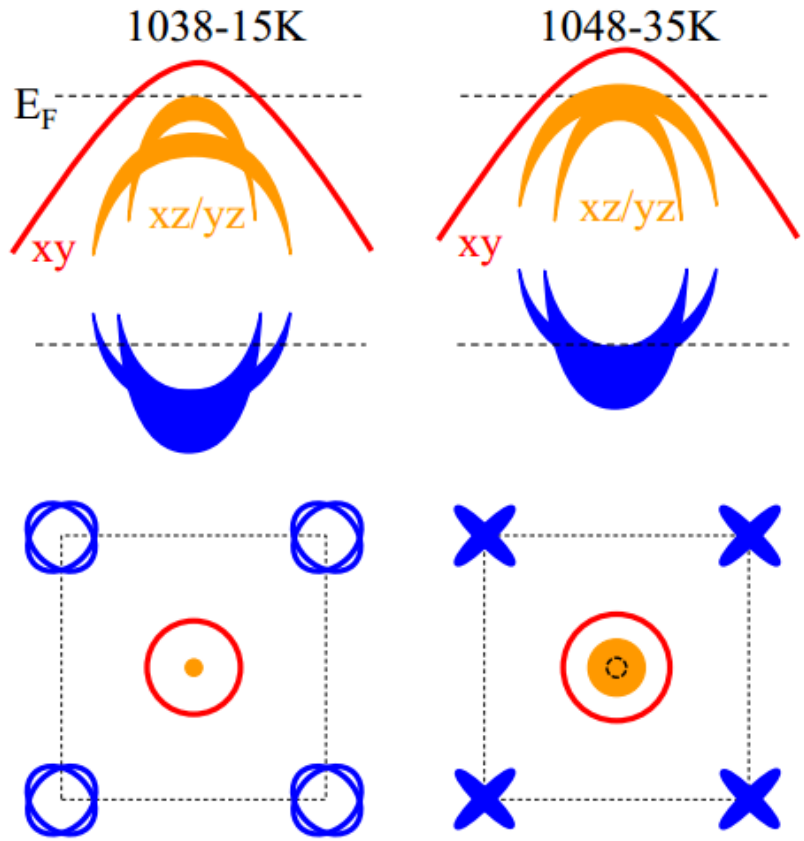


D. V. Evtushinsky arXiv:1211.4593

$(CaFe_{0.95}Pt_{0.05}As)_{10}Pt_3As_8$ **"10 3 8" – 15K**

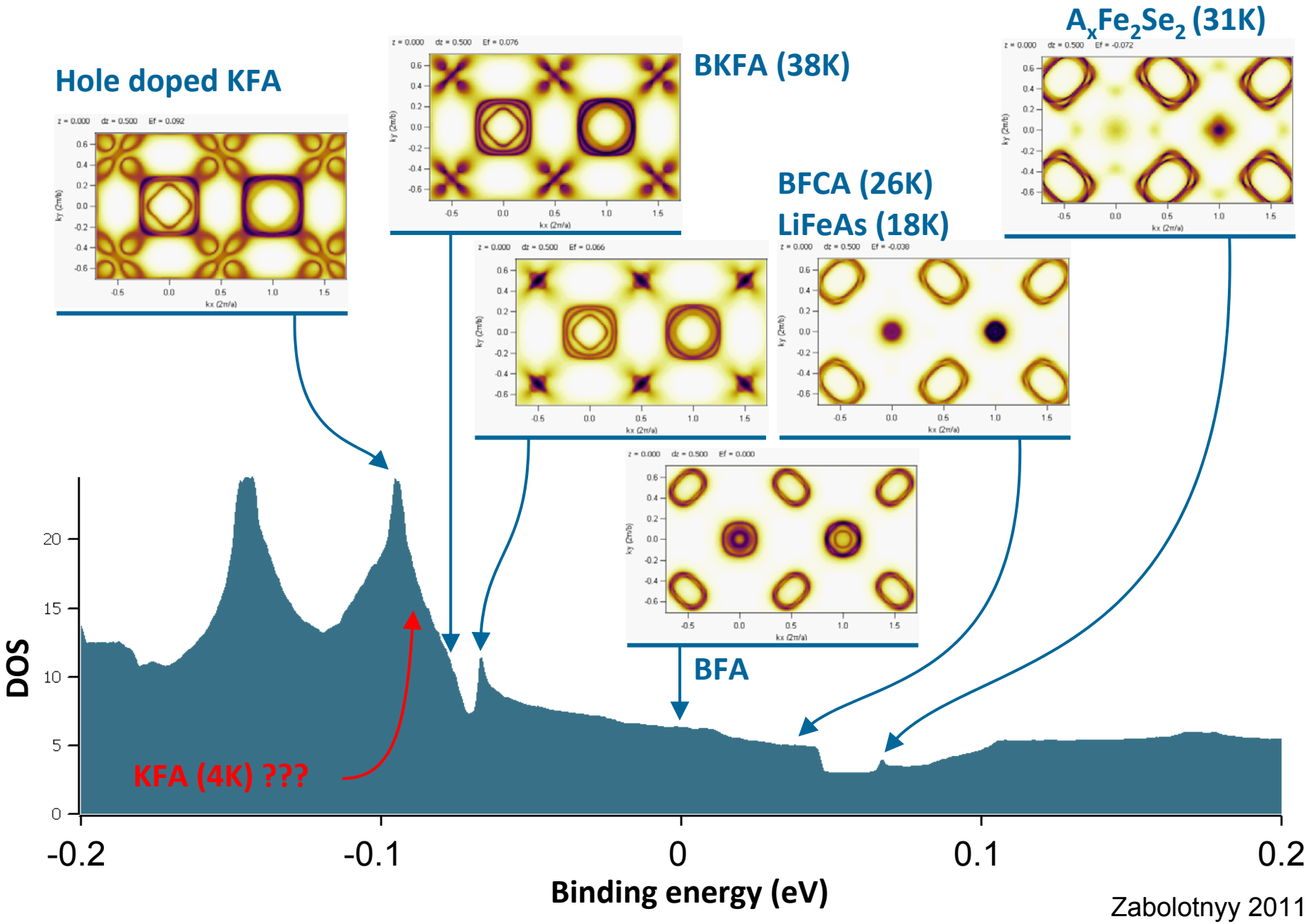
$(CaFeAs)_{10}Pt_{3.58}As_8$ **"10 4 8" – 35K**





S.Thirupathaiah arXiv:1307.1608

BFA: density of states



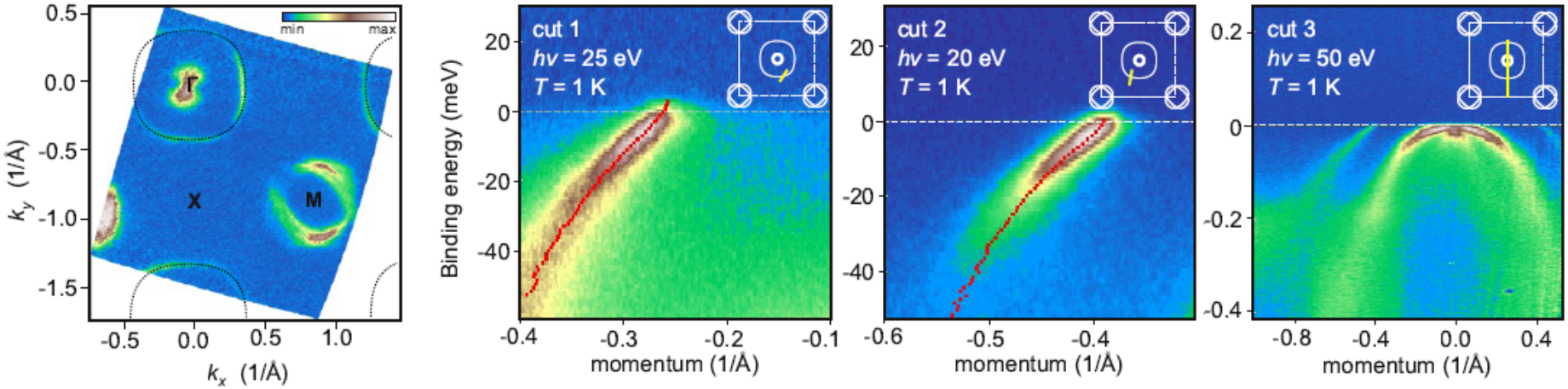
Zabolotnyy 2011

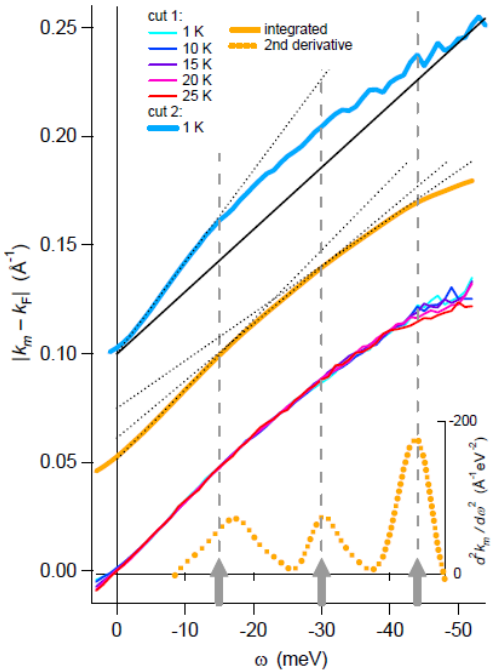
- **The band structure of Fe-SC is well captured by LDA but do not take it too literally. The calculated Fermi surface is usually bad starting point for theory.**
- **Main contributors to SC are dxz,yz electrons and Tc for different compounds seems to correlate with the position of the Van Hove singuliarities (Lifshitz transitions) for the xz- and yz-bands.**

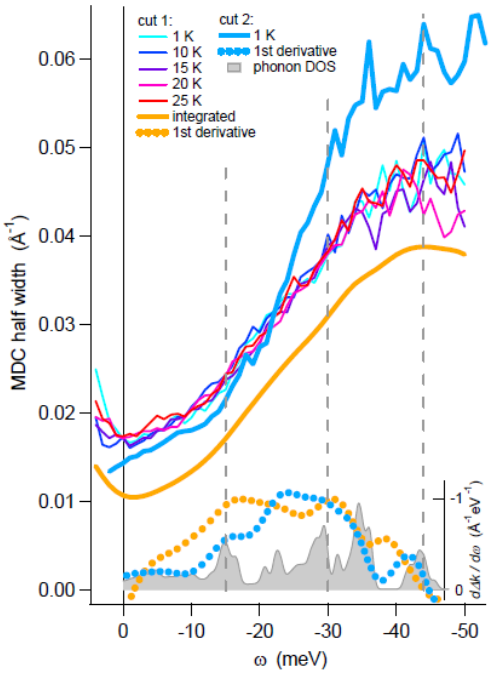
Self-energy in Fe-SC

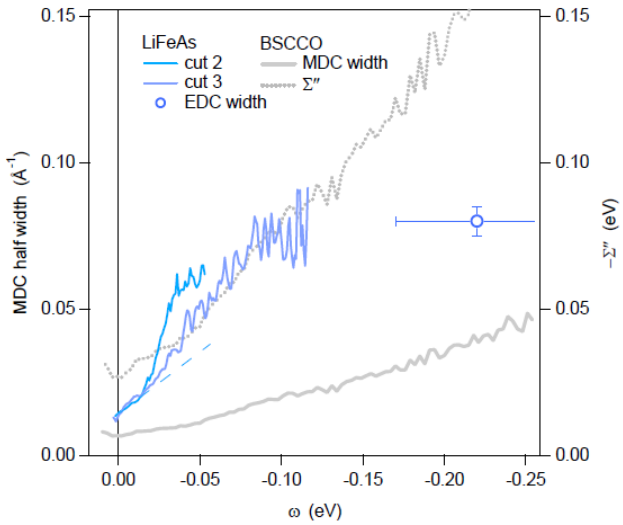
- crystal quality
- 3D
- lack of manpower

LiFeAs: renormalization





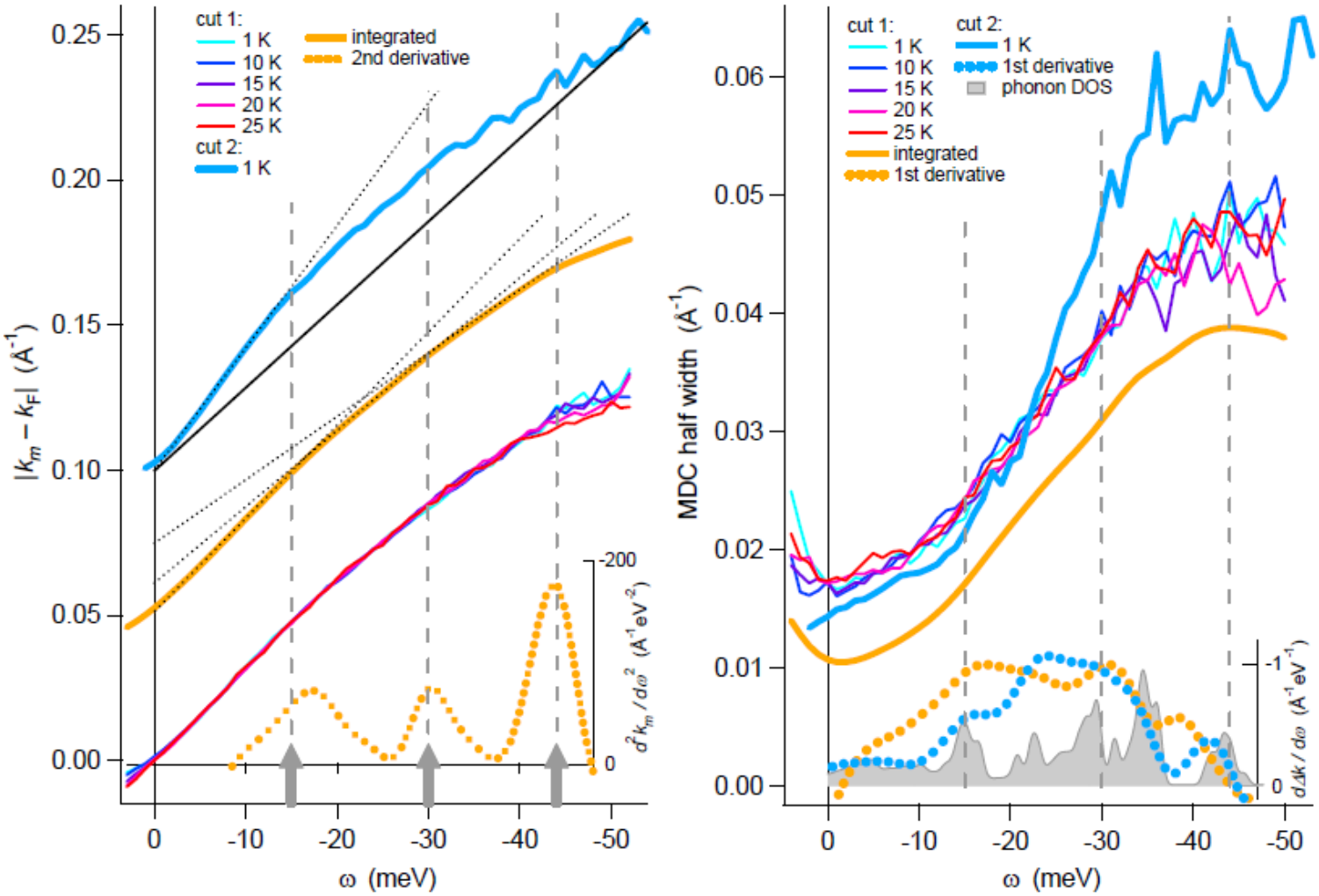




$$\lambda = \lambda_{el} + \lambda_{ph} = 2 + 1.38$$

Kordyuk *PRB* 2010

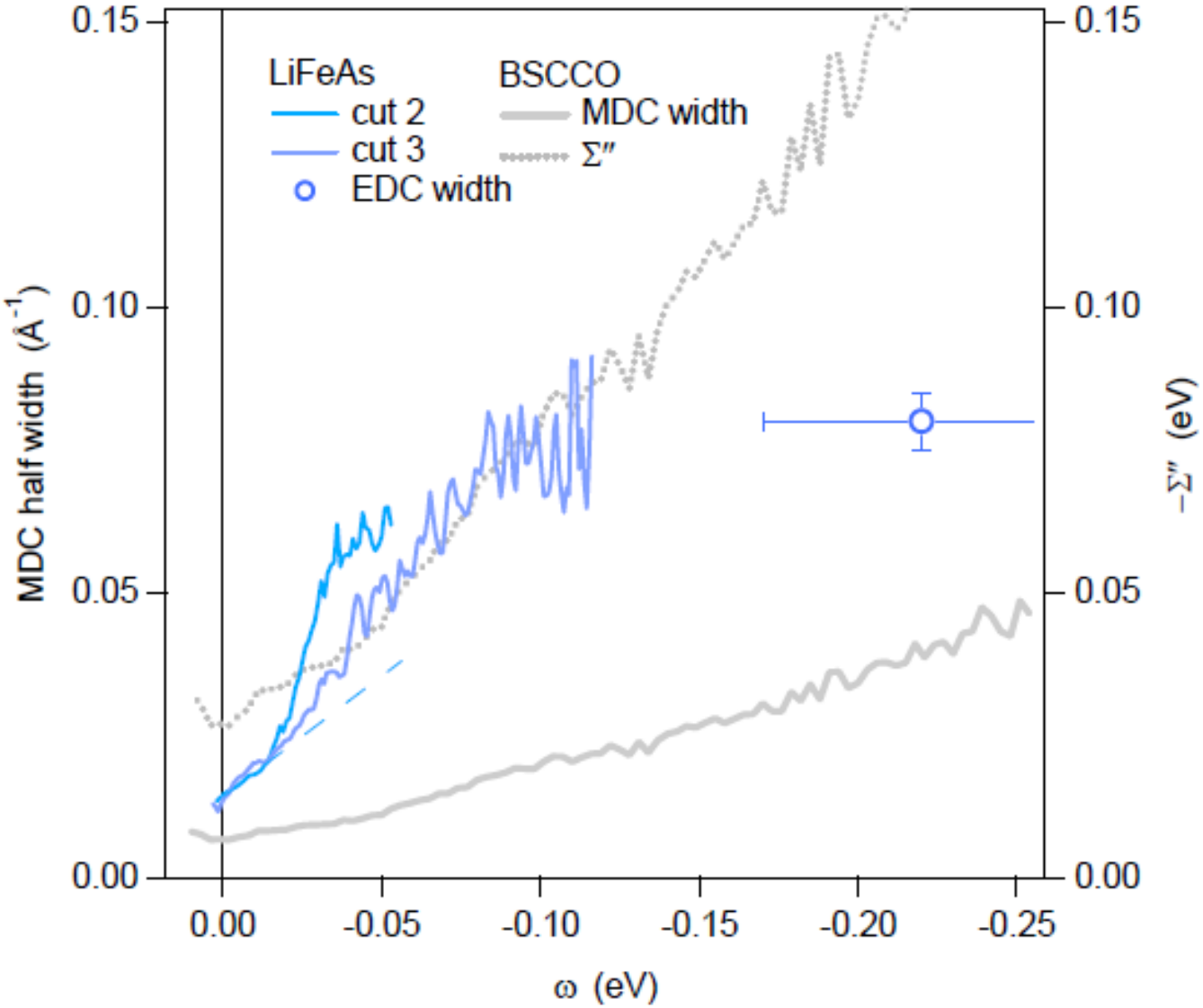
LiFeAs: renormalization



$$\lambda = \lambda_{el} + \lambda_{ph} = 2 + 1.38$$

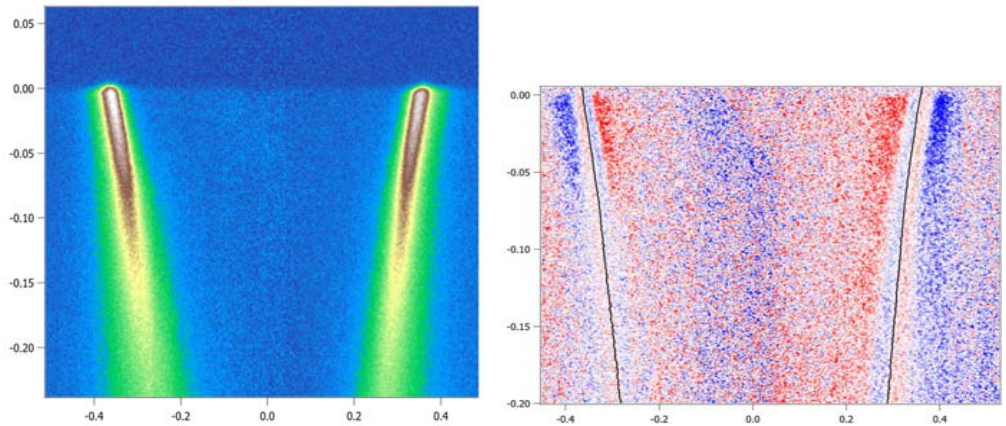
Kordyuk *PRB* 2010

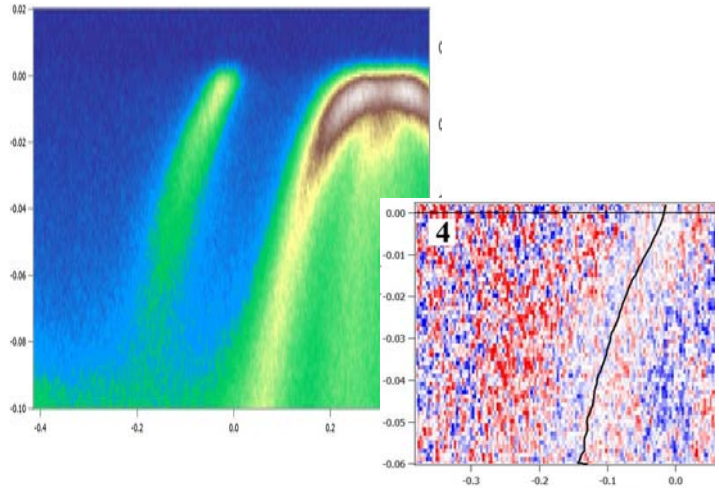
LiFeAs: renormalization

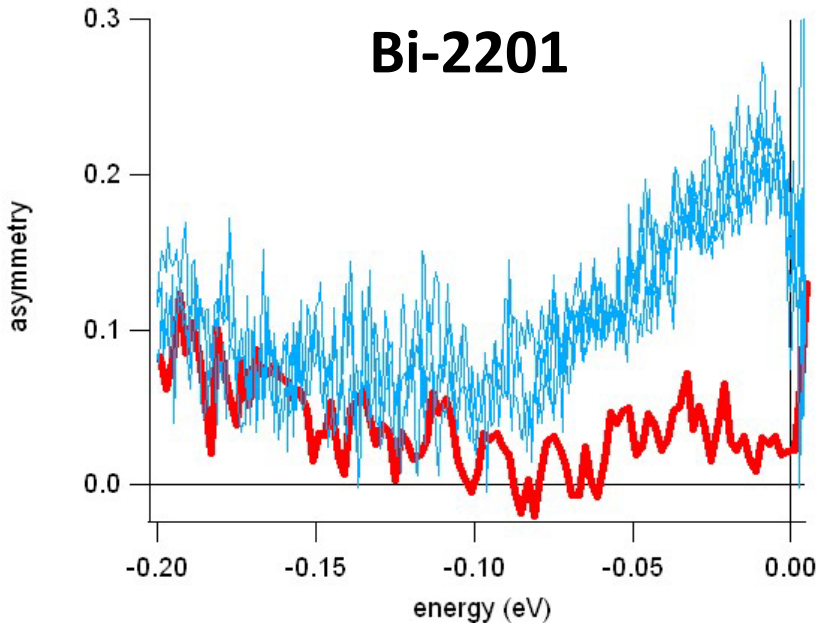


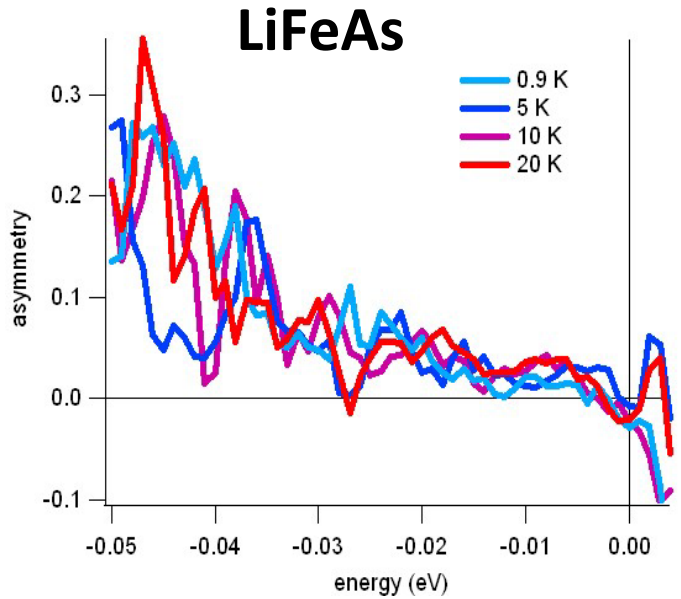
Kordyuk *PRB* 2010

MDC asymmetry = k-dependent self-energy









Kushnirenko 2013 (see poster)

Cuprates vs ferropnictides

	Cu-SC	Fe-SC
band structure	simple (1 band, split)	complex (5 bands)
renormalization	k-dependent	band dependent
$1+\lambda$ (ω cutoff)	k-dependent 2 (0.5 eV)	>4 (50 meV) 3 (1.5 eV)
SC gap	k-dependent	band dependent
pseudogap	k-dependent	no
main interaction	SF	(phonons + SF) *multi-bands

Collaboration

IMP
Daniil Evtushinsky
Alexander Plyushchay
Eugen Kushnirenko
Michael Procovovich
…

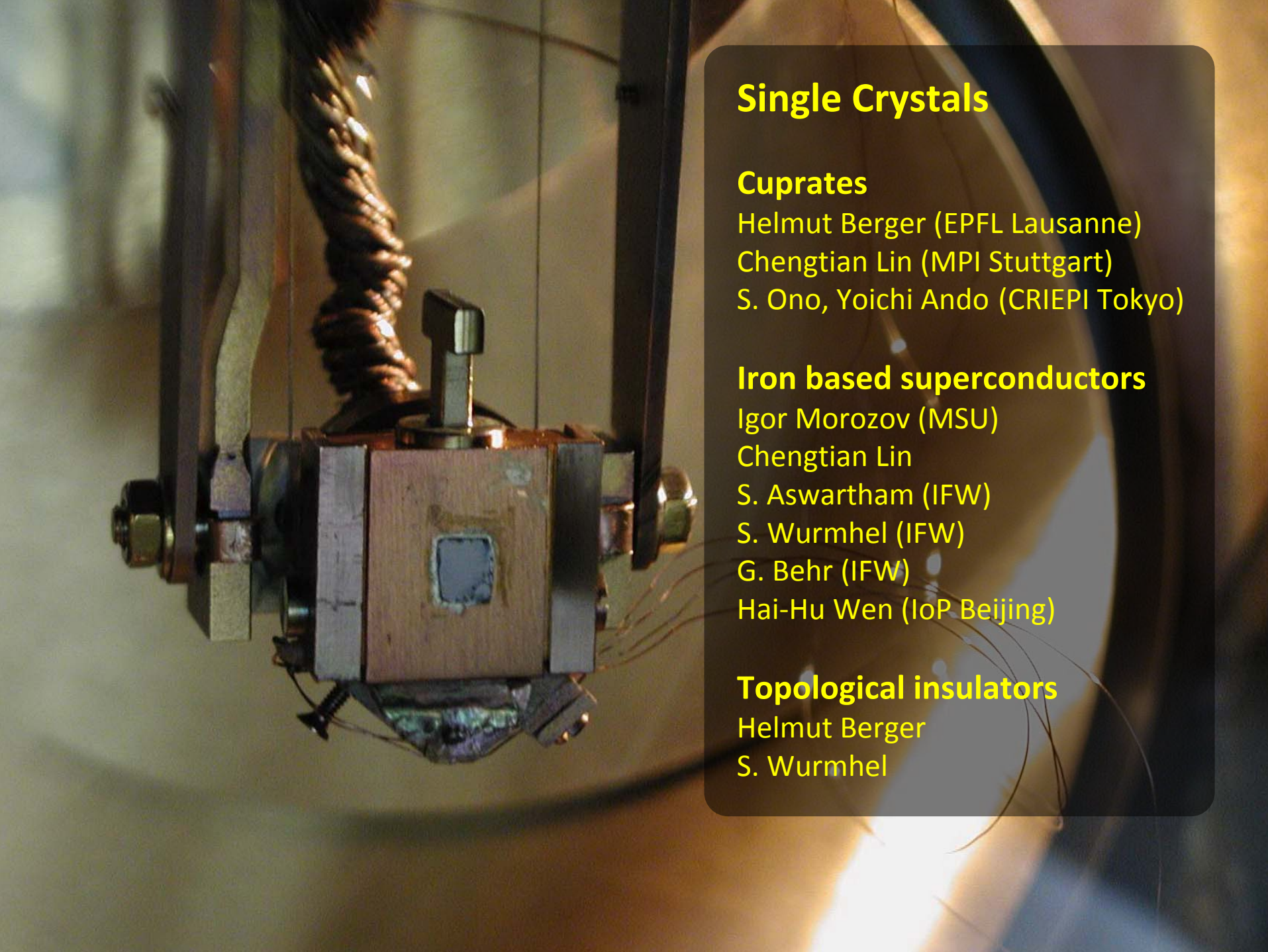
ARPES, IFW Dresden
Sergey Borisenko
Volodymyr Zabolotny
Daniil Evtushinsky
Timur Kim
Dmytro Inosov
Andreas Koitzsch
Roland Hübel
Jörg Fink
…

ARPES Worldwide
Mark Golden (UvA)
Toni Valla (BNL)
…

Neutron Scattering
Vladimir Hinkov
Bernhard Keimer
Dmytro Inosov

STM & Transport
Cristian Hess
Bernd Buehner
Alexey Pan
Vladimir Karbovskii

Theory
Alexander Yaresko
Eugene Krasovskii
Thomas Dahm
Doug Scalapino
Andrey Chubukov
Ilya Eremin



Single Crystals

Cuprates
Helmut Berger (EPFL Lausanne)
Chengtian Lin (MPI Stuttgart)
S. Ono, Yoichi Ando (CRIEPI Tokyo)

Iron based superconductors
Igor Morozov (MSU)
Chengtian Lin
S. Aswartham (IFW)
S. Wurmhel (IFW)
G. Behr (IFW)
Hai-Hu Wen (IoP Beijing)

Topological insulators
Helmut Berger
S. Wurmhel

Synchrotron Light

BESSY (Berlin)

Emile Rienks
Rolf Follath
Andrei Varykhalov
Serguei Molodtsov

SLS (PSI Villigen)

Ming Shi
Vladimir Strocov
Luc Patthey
Joel Mesot

ELETTRA (Trieste)

Alexei Barinov
Pavel Dudin
Stefano Turchini


Thank You!