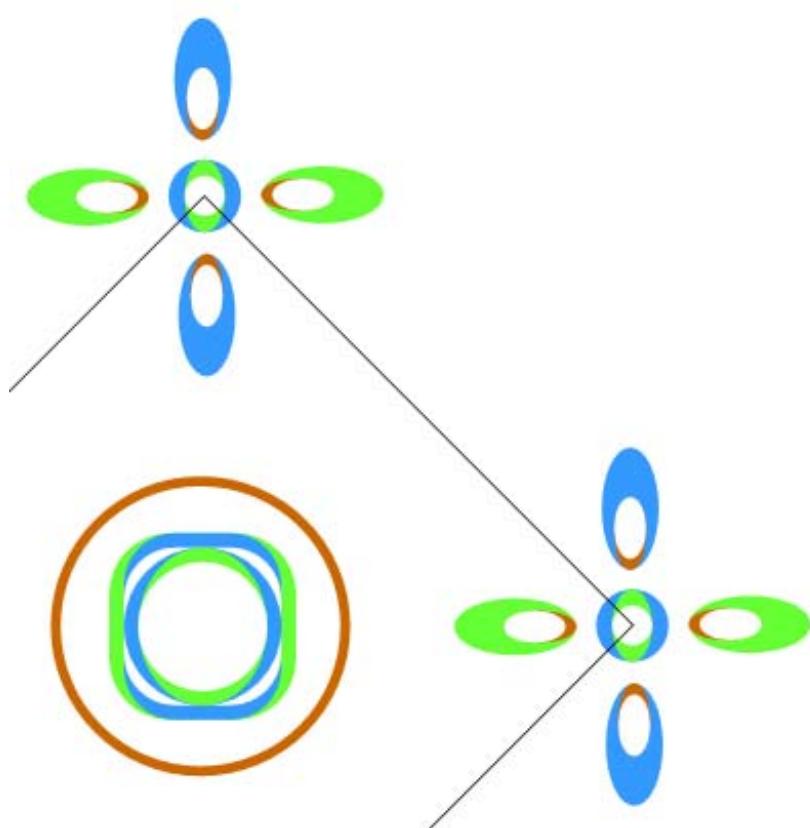


Electronic band structure of ferro-pnictide superconductors (FPS)



Alexander Kordyuk
IFW Dresden & IMP Kiev

FPS'11
Zvenigorod, 03.10.2011

Authors and Collaborations



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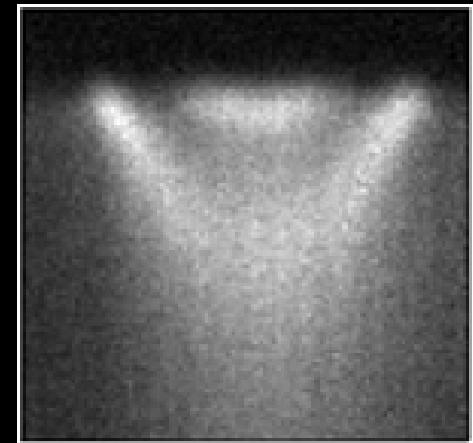
DFG Research Unit 538
and priority program
SPP 1458

Plan

- ARPES on FPS
- Band structure of 111 and 122
- Which electrons do superconductivity
- ... and why?

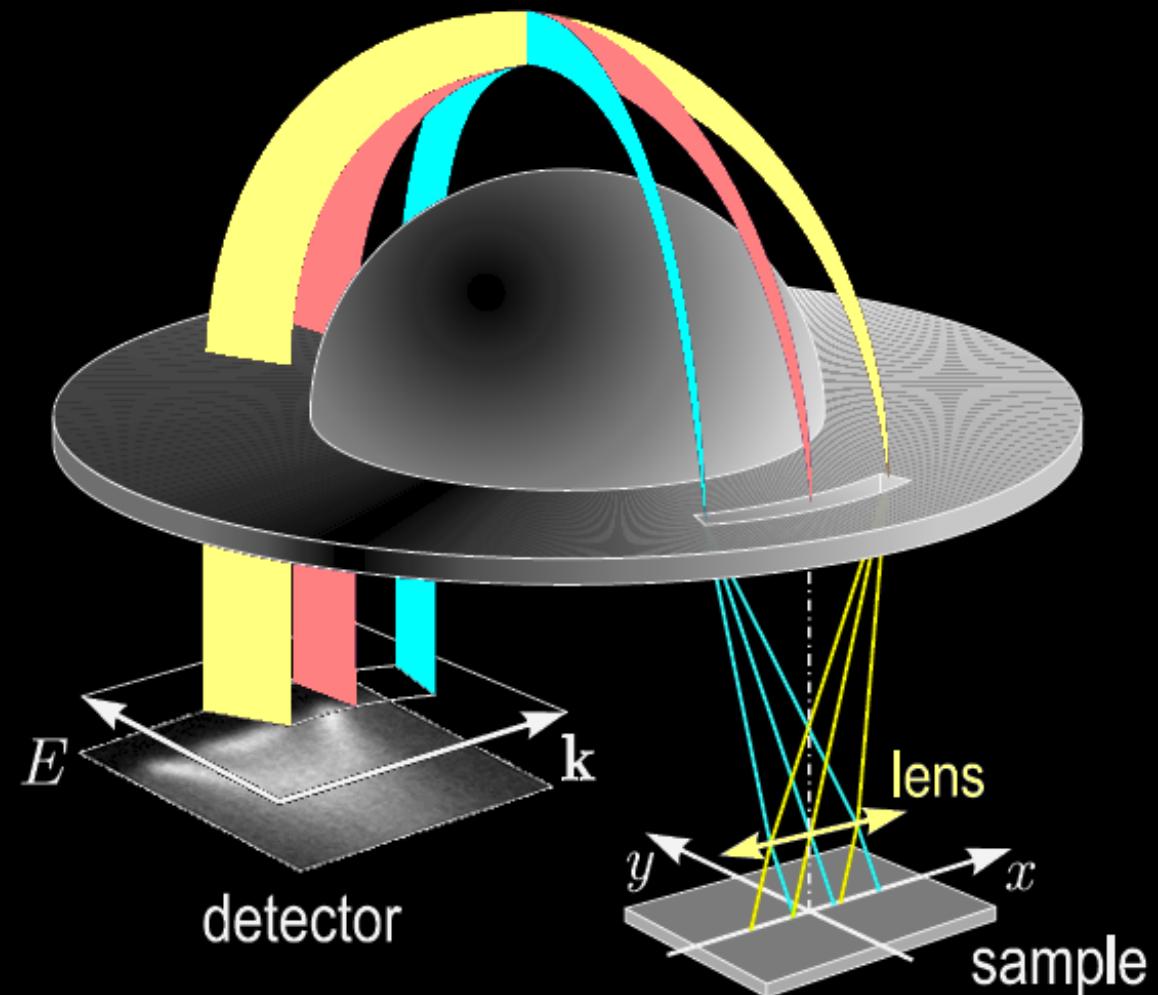
Photoelectric effect + electron analyser

ARPES Image

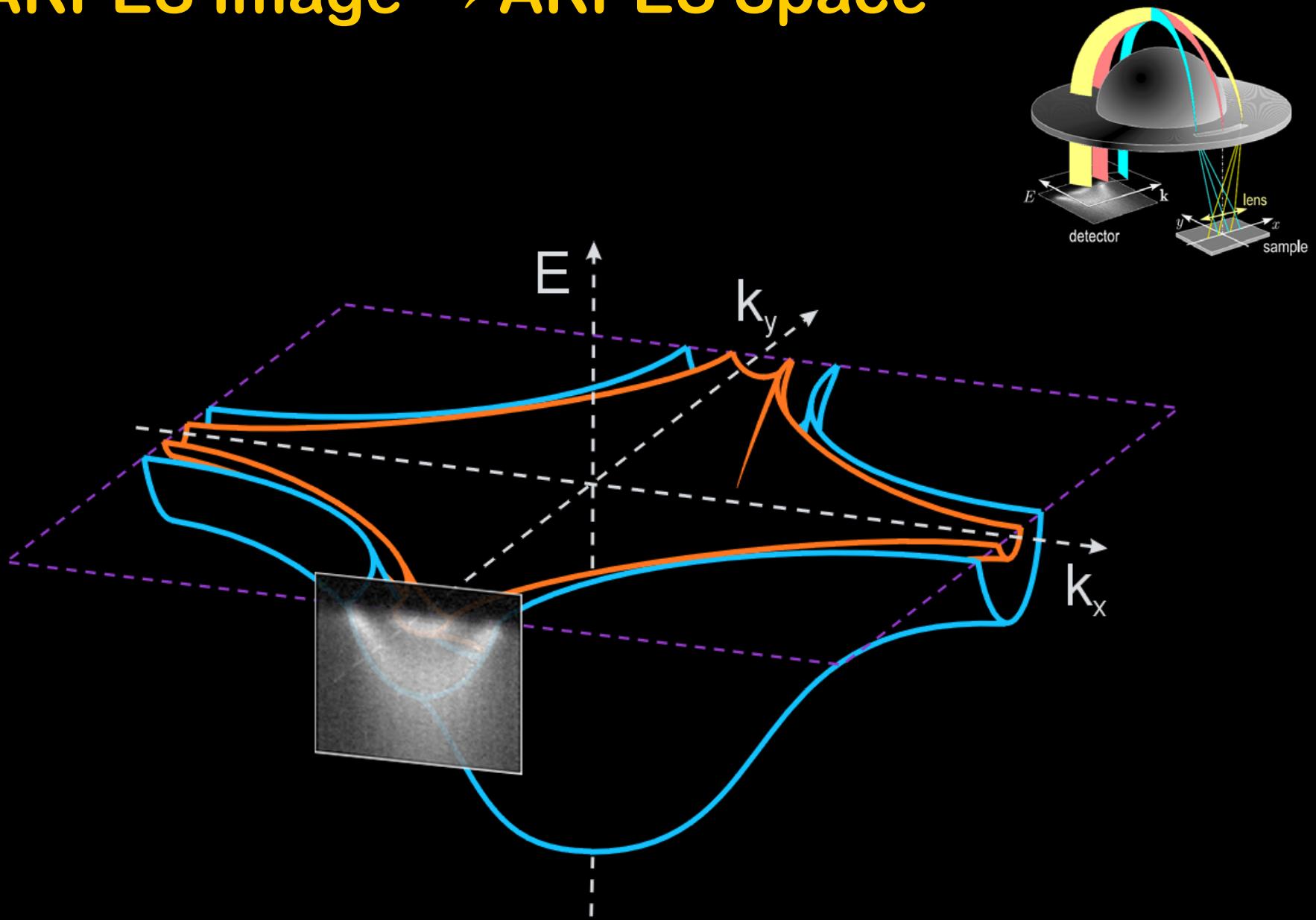


energy

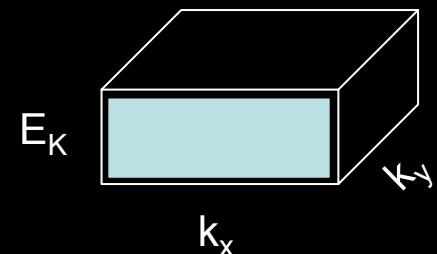
angle / momentum



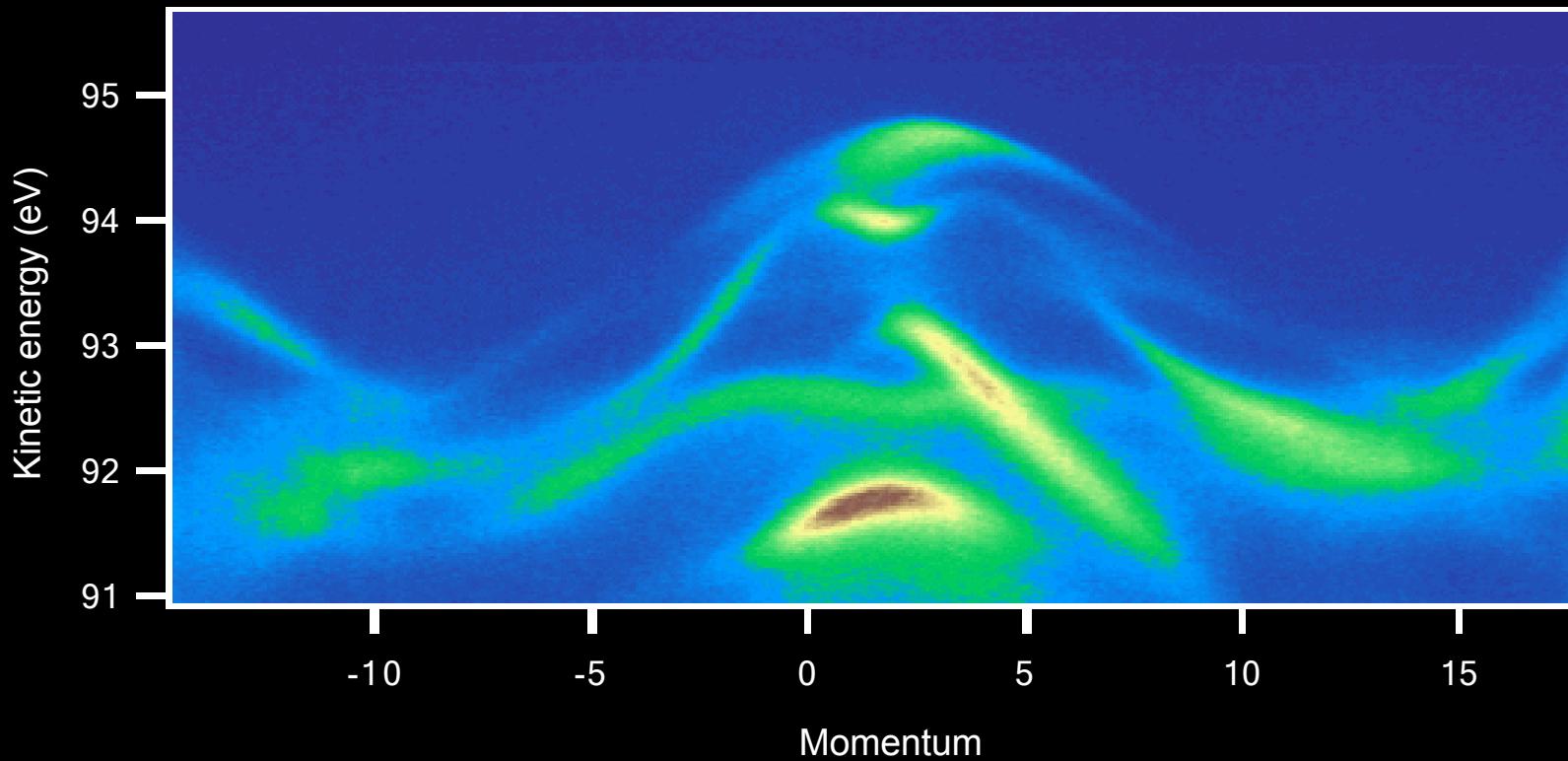
ARPES Image → ARPES Space



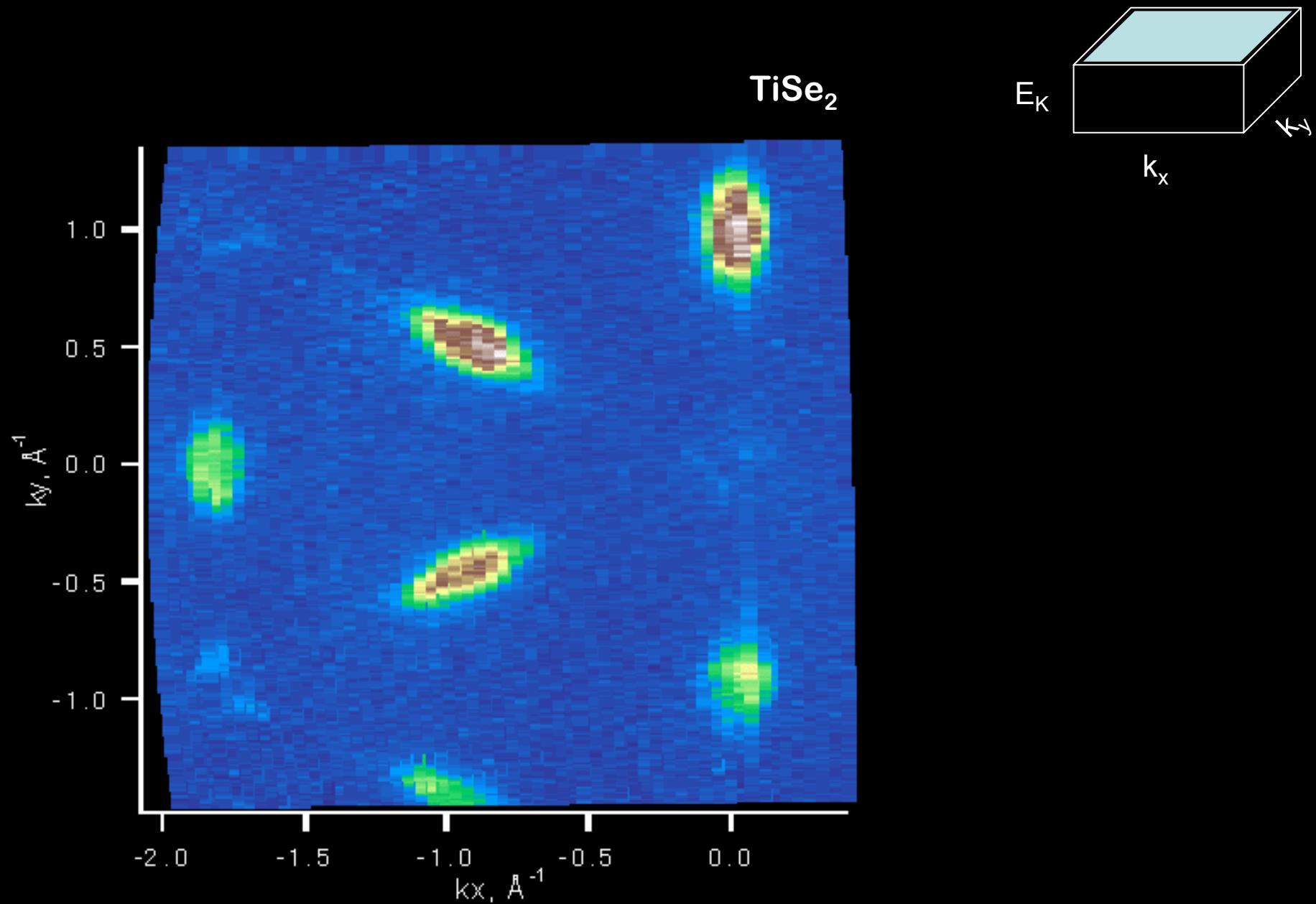
Momentum-energy space



TiSe_2

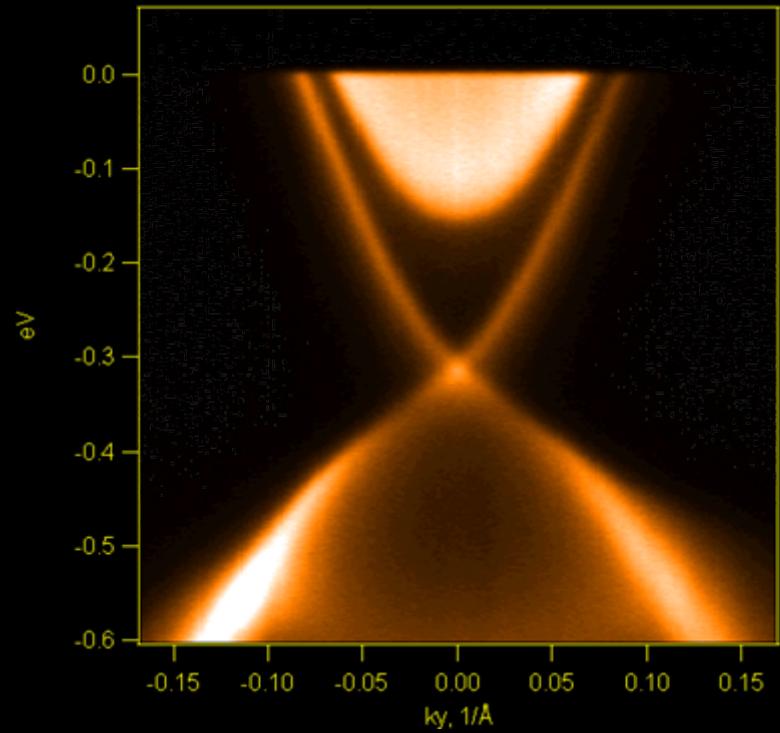
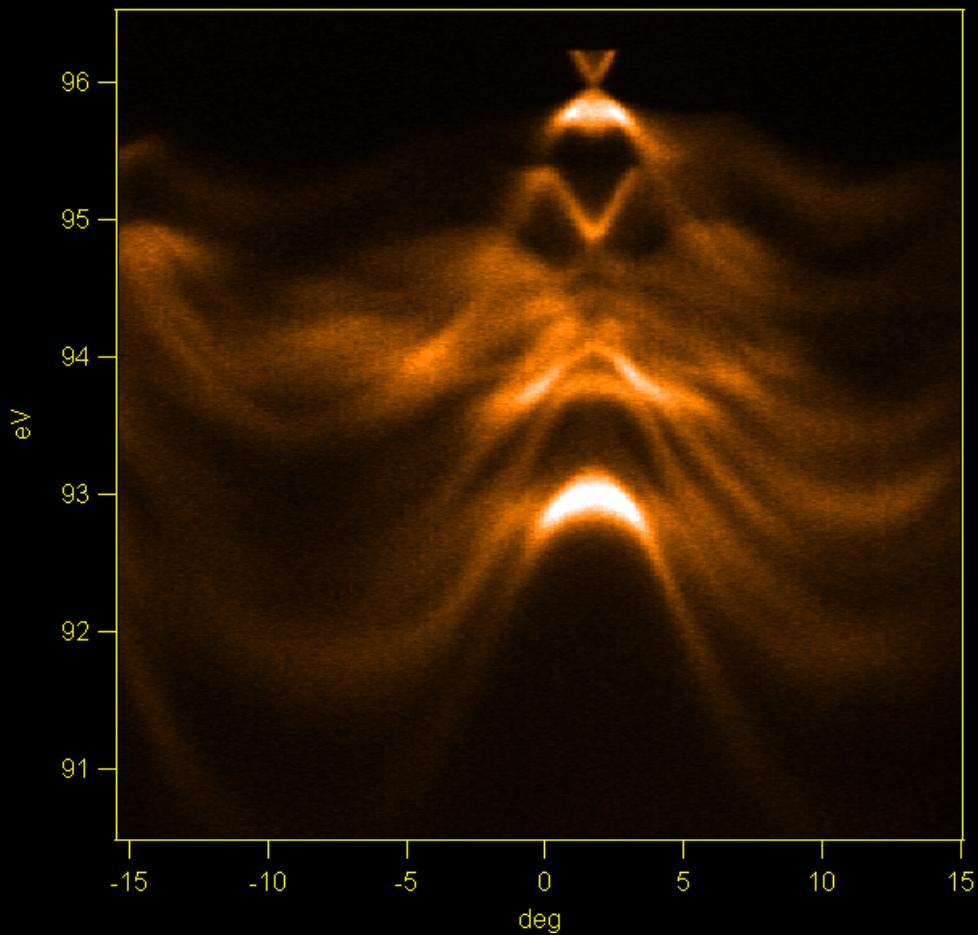


Fermi surface (energy distribution) map

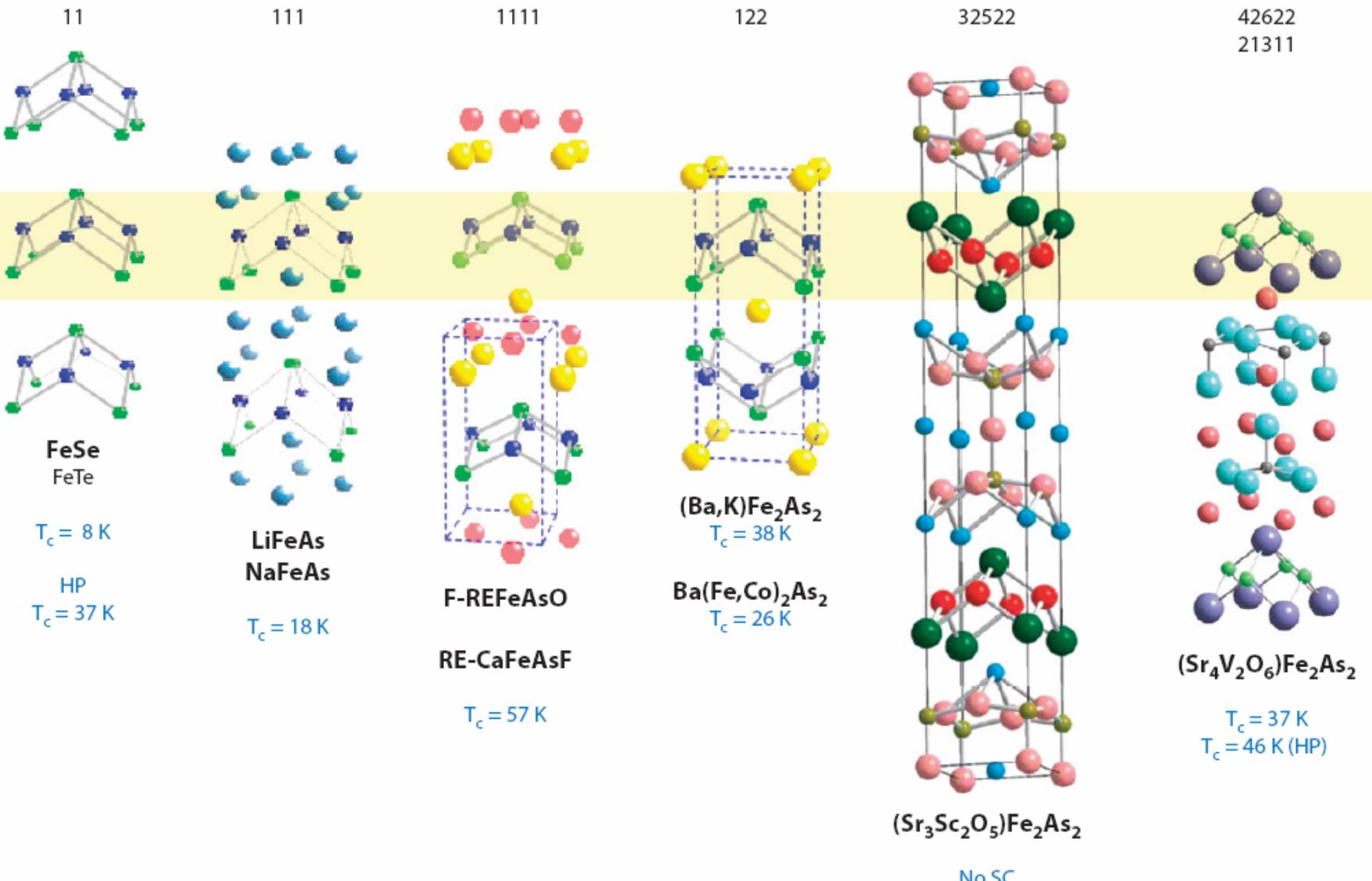


Surface vs Bulk

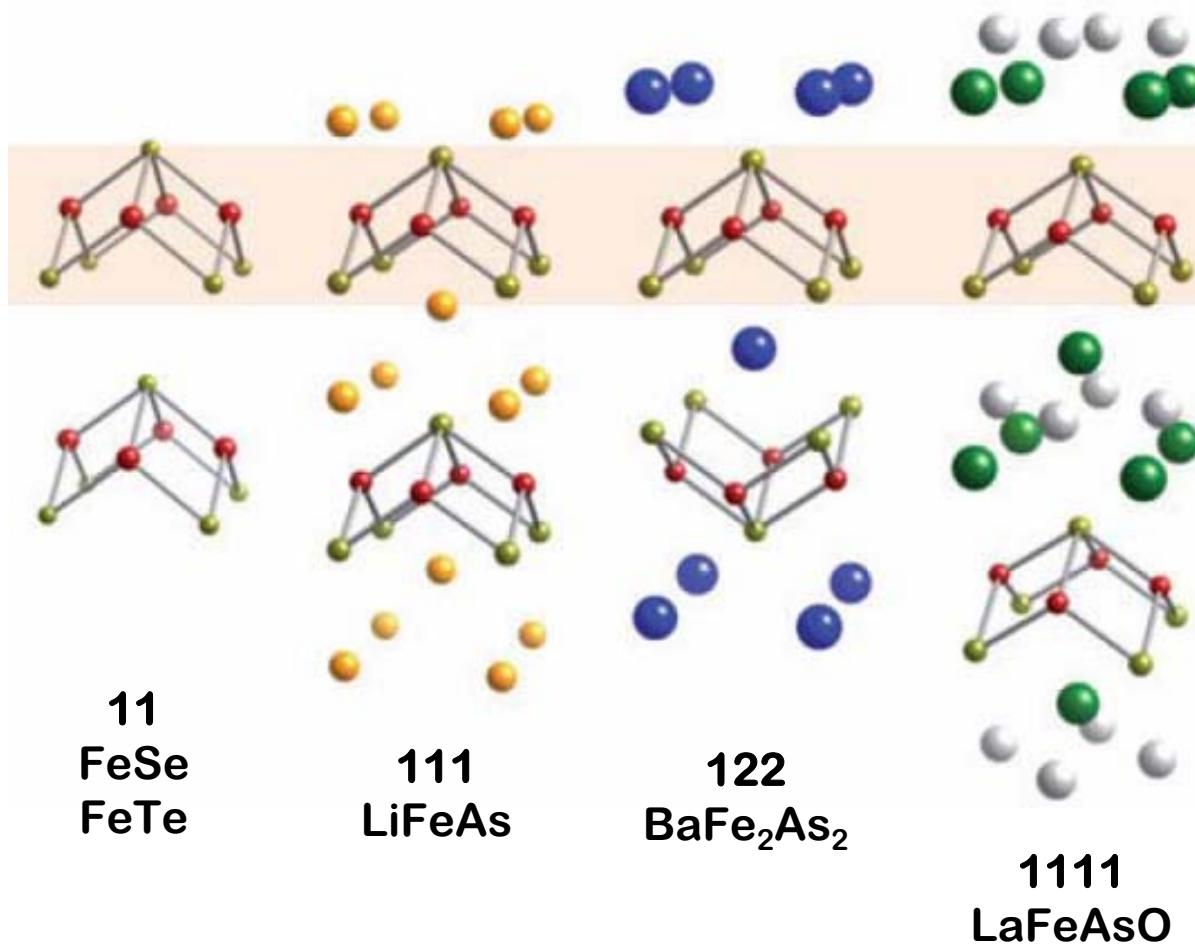
Bi_2Se_3



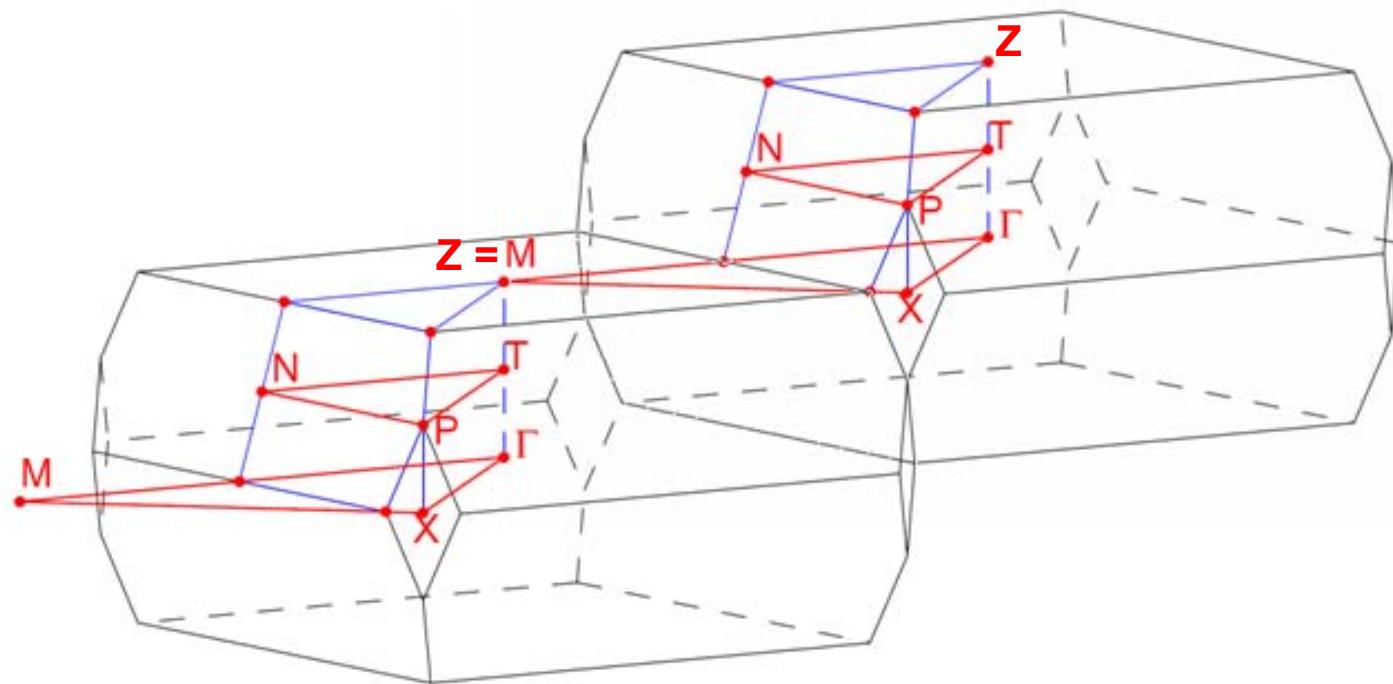
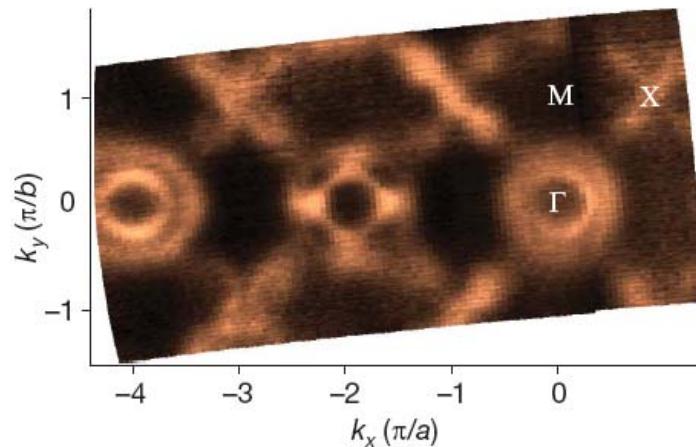
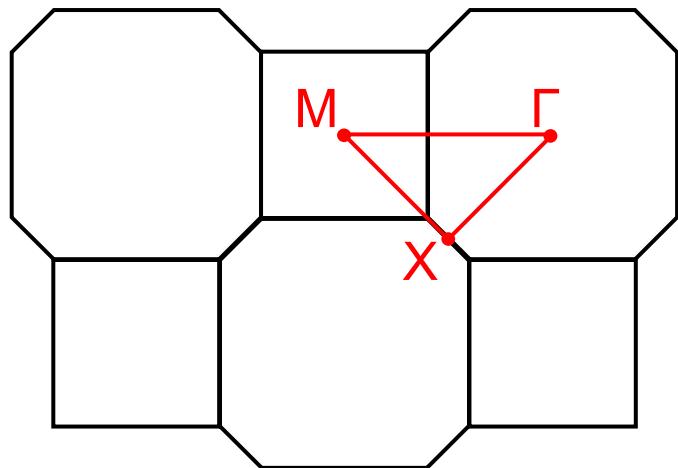
Iron-based superconductors



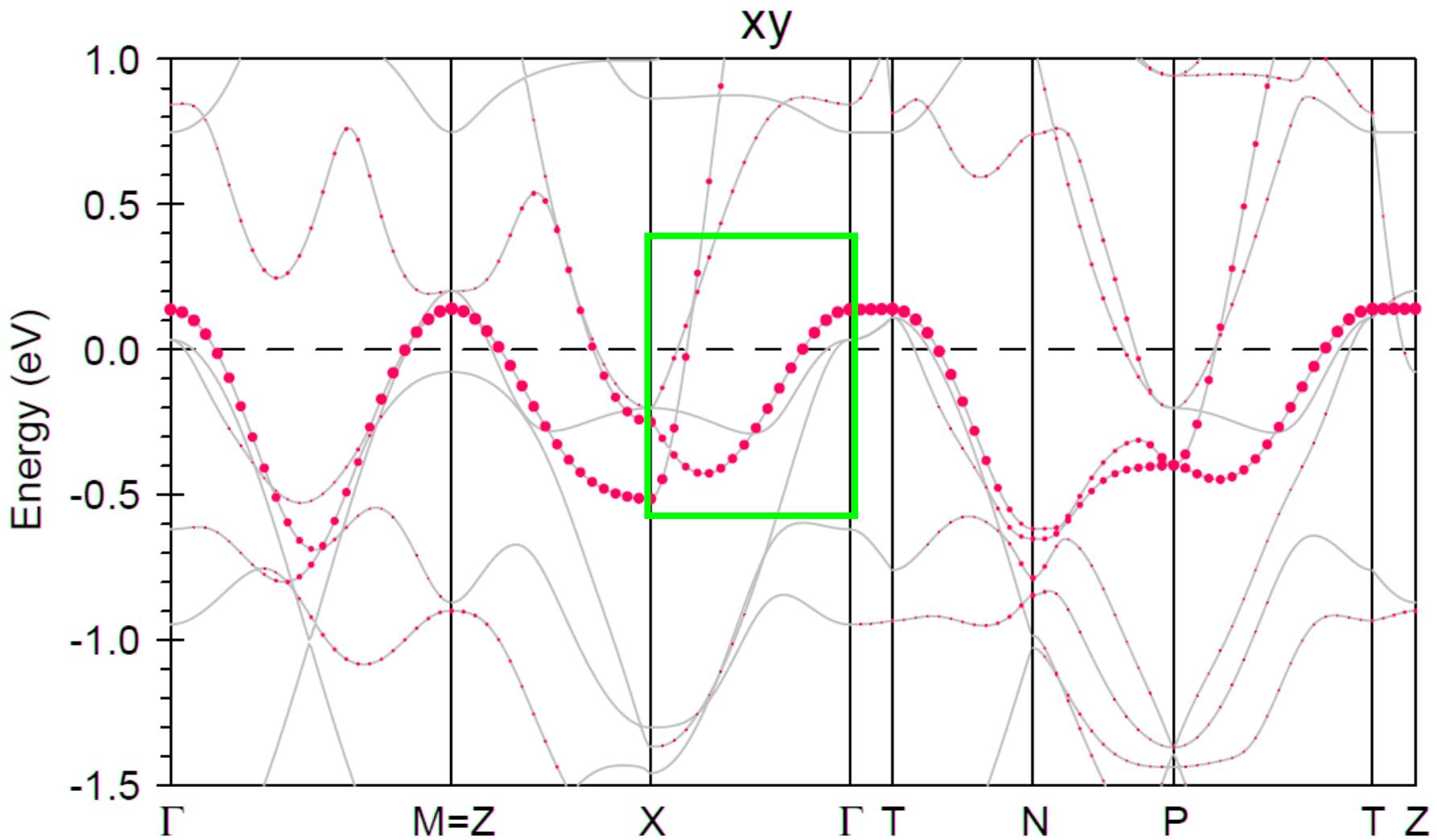
Iron-based superconductors



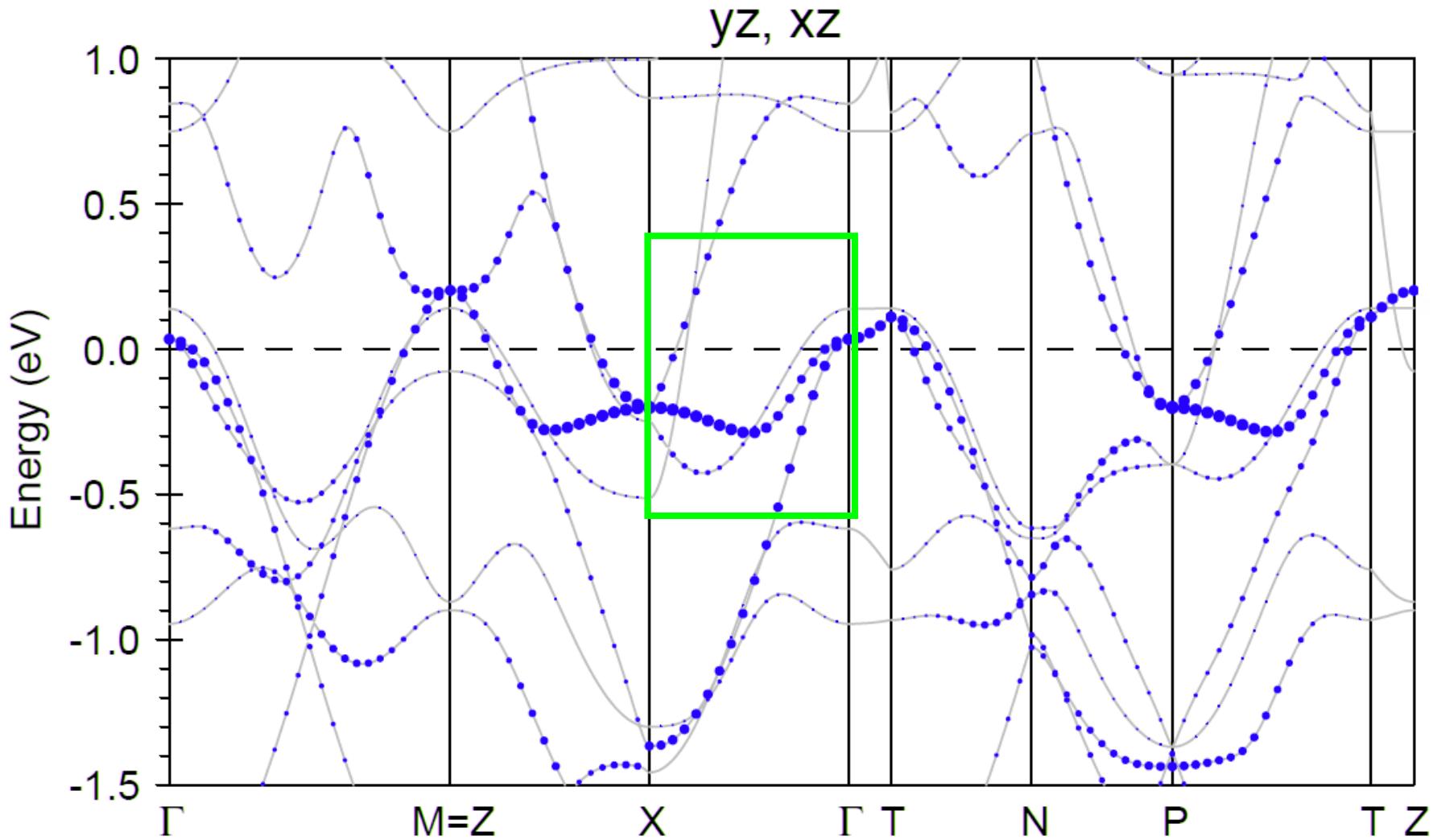
122: truncated square tiling



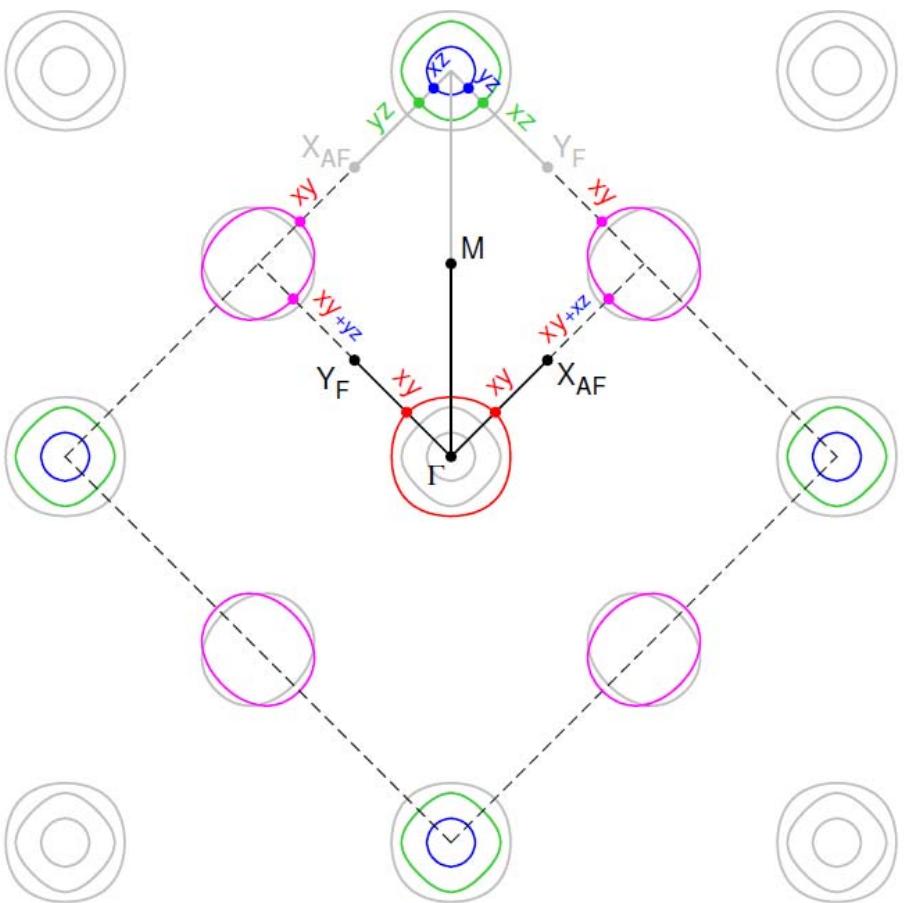
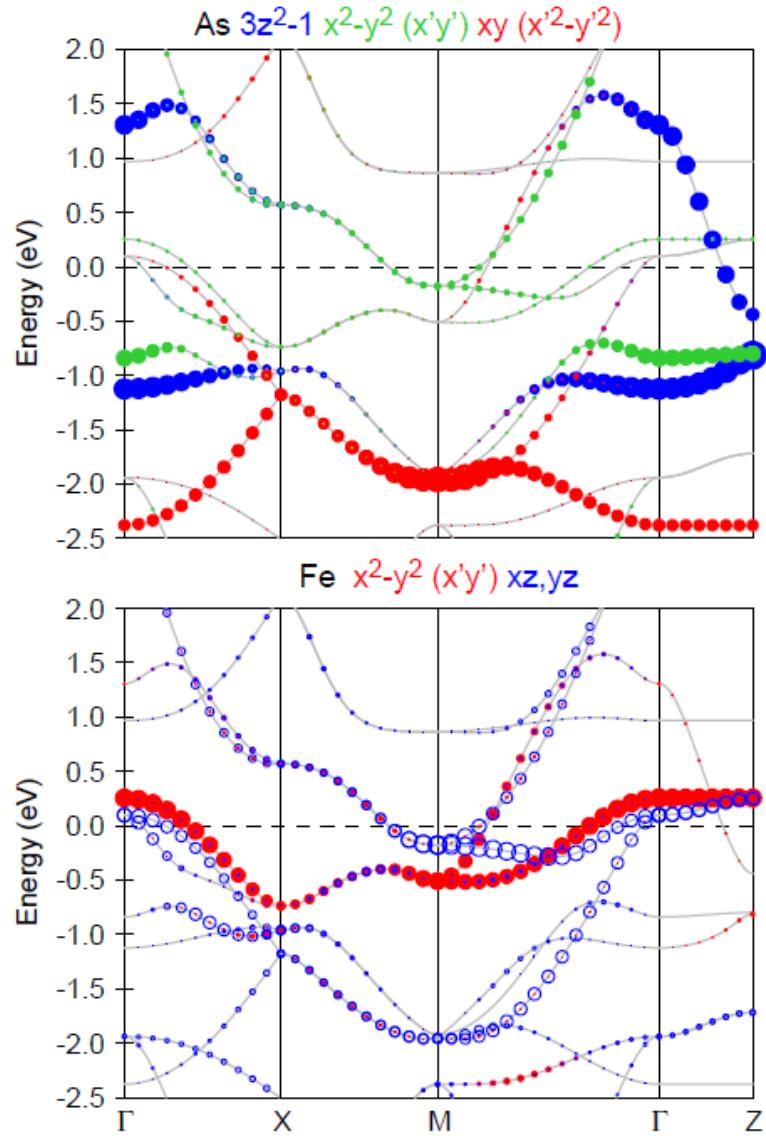
Band structure of 122 (BFA)



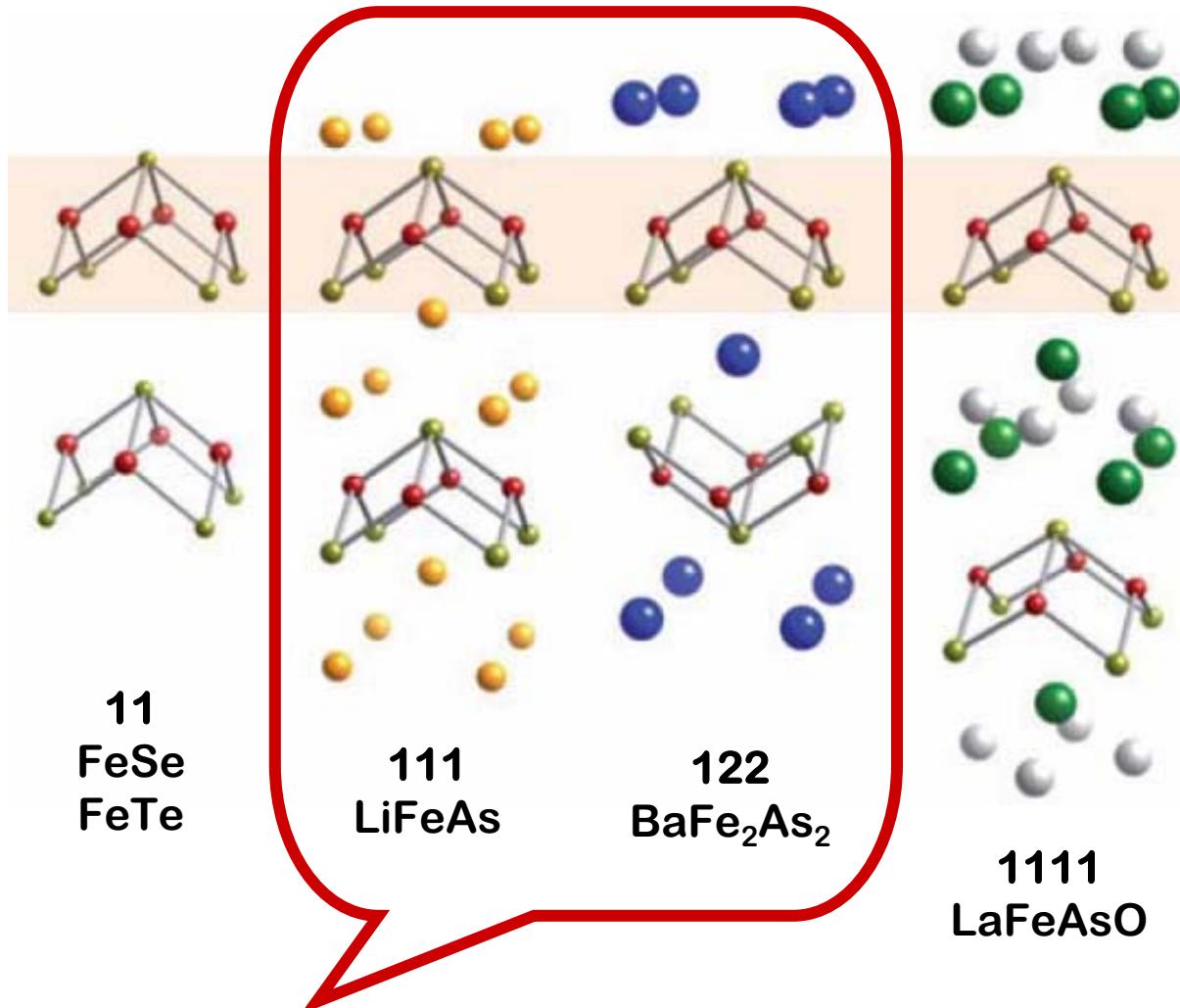
Band structure of 122 (BFA)



Band structure of FPS



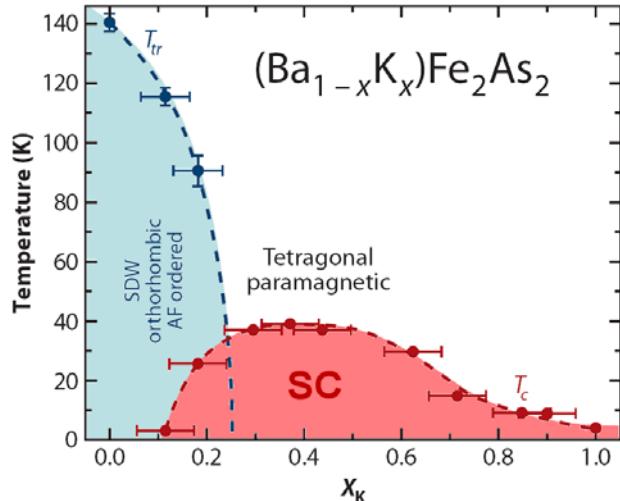
Iron-based superconductors



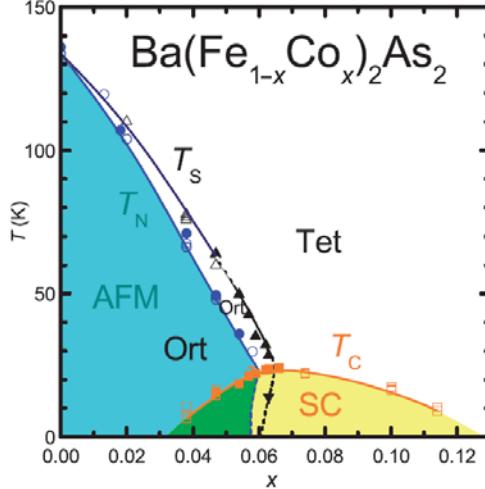
ARPESable

Paglione & Greene, *Nat. Phys.* (2010)

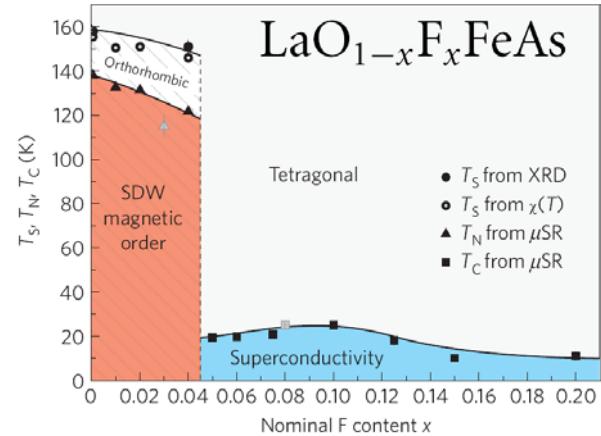
Phase diagrams



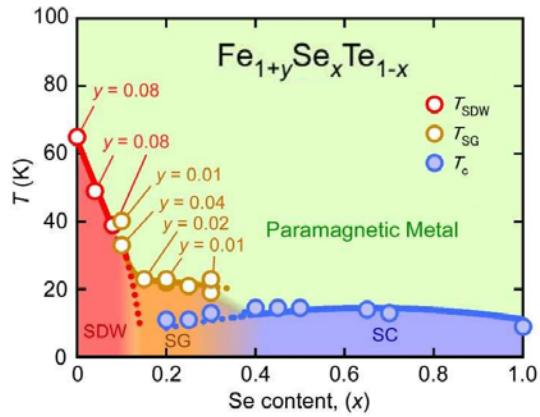
H.-H.Wen & S.Li [Annu. Rev. Cond. Mat. Phys. 2011](#)



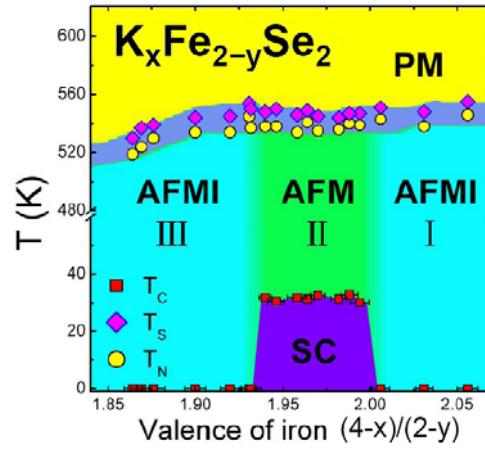
S.Nandi *et al.* [PRL 2010](#)



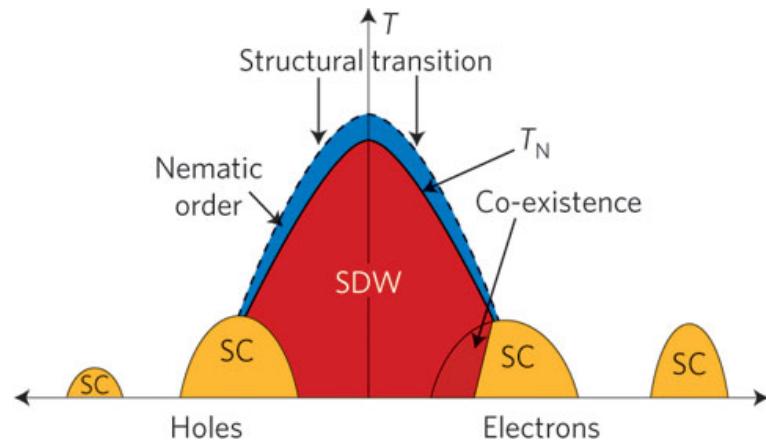
H.Luetkens *et al.* [Nature Mat. 2009](#)



N.Katayama *et al.* [arXiv:1003.4525](#)

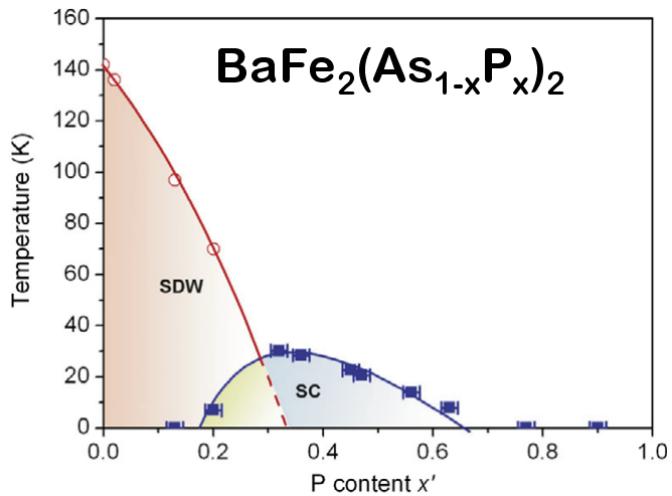


Y.J.Yan *et al.* [arXiv:1104.4941](#)

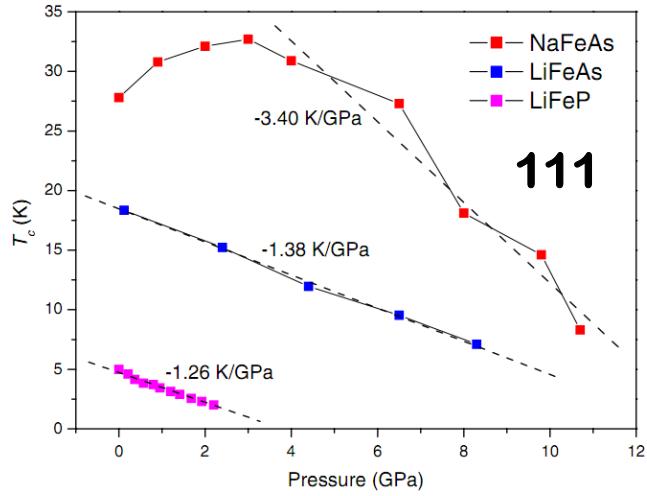


Basov & Chubukov [Nature Phys. 2011](#)

Phase diagrams



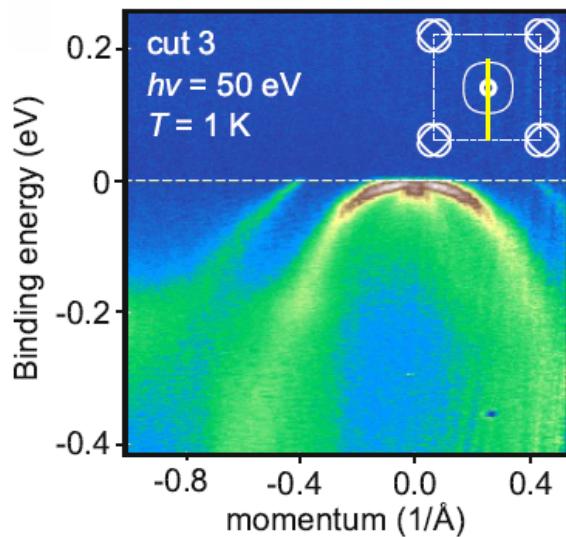
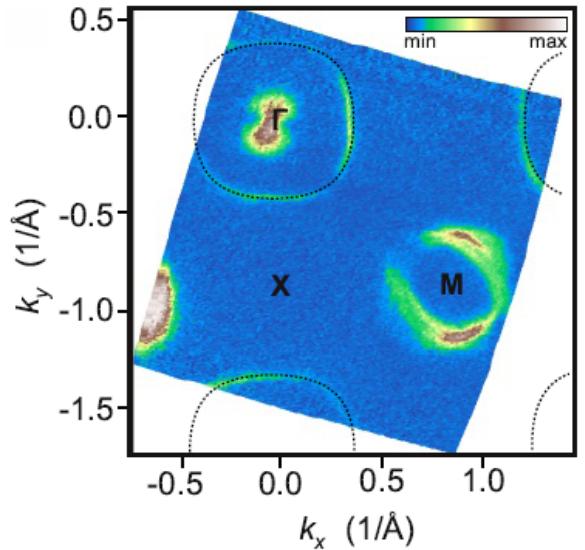
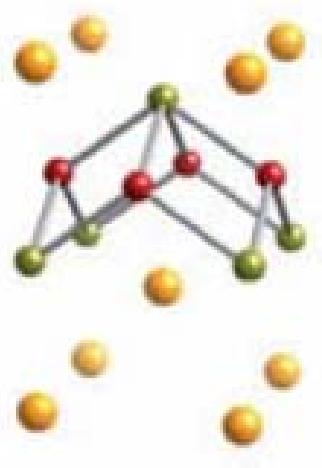
S.Jiang *et al.* [J.Phys.Cond.Matt. 2009](#)



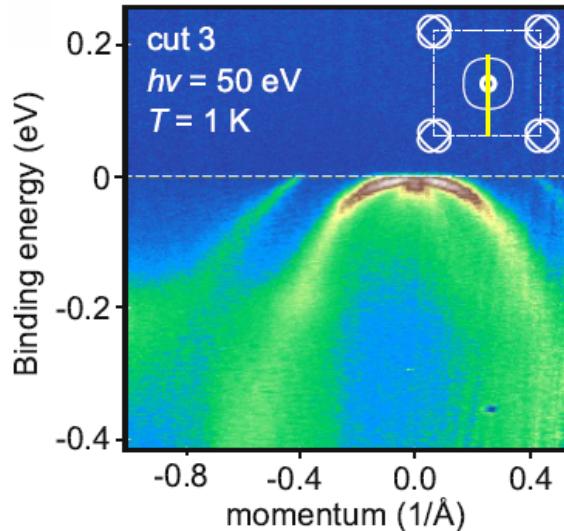
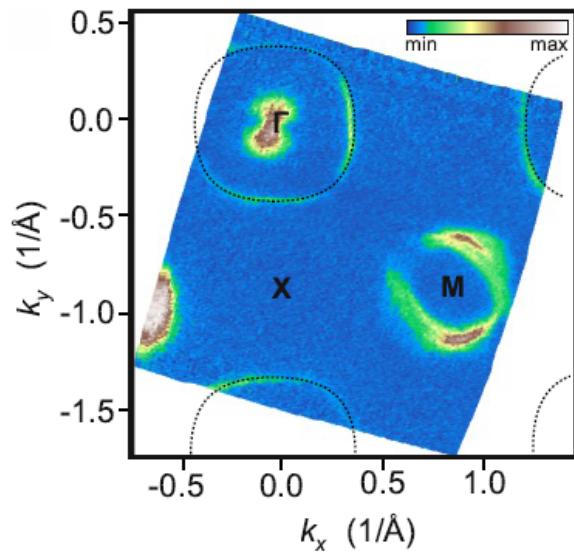
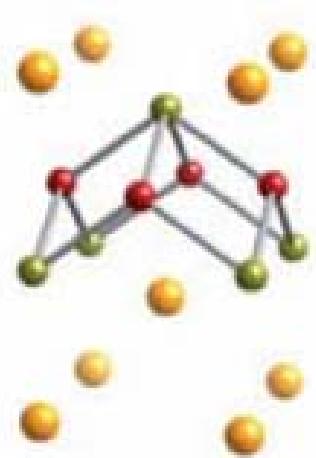
X.C.Wang *et al.* [High Pressure Research 2011](#)

111

LiFeAs ($T_c = 18$ K, non-magnetic)
NaFeAs ($T_c = 9\text{-}26$ K, $T_{AF} = 40$ K)

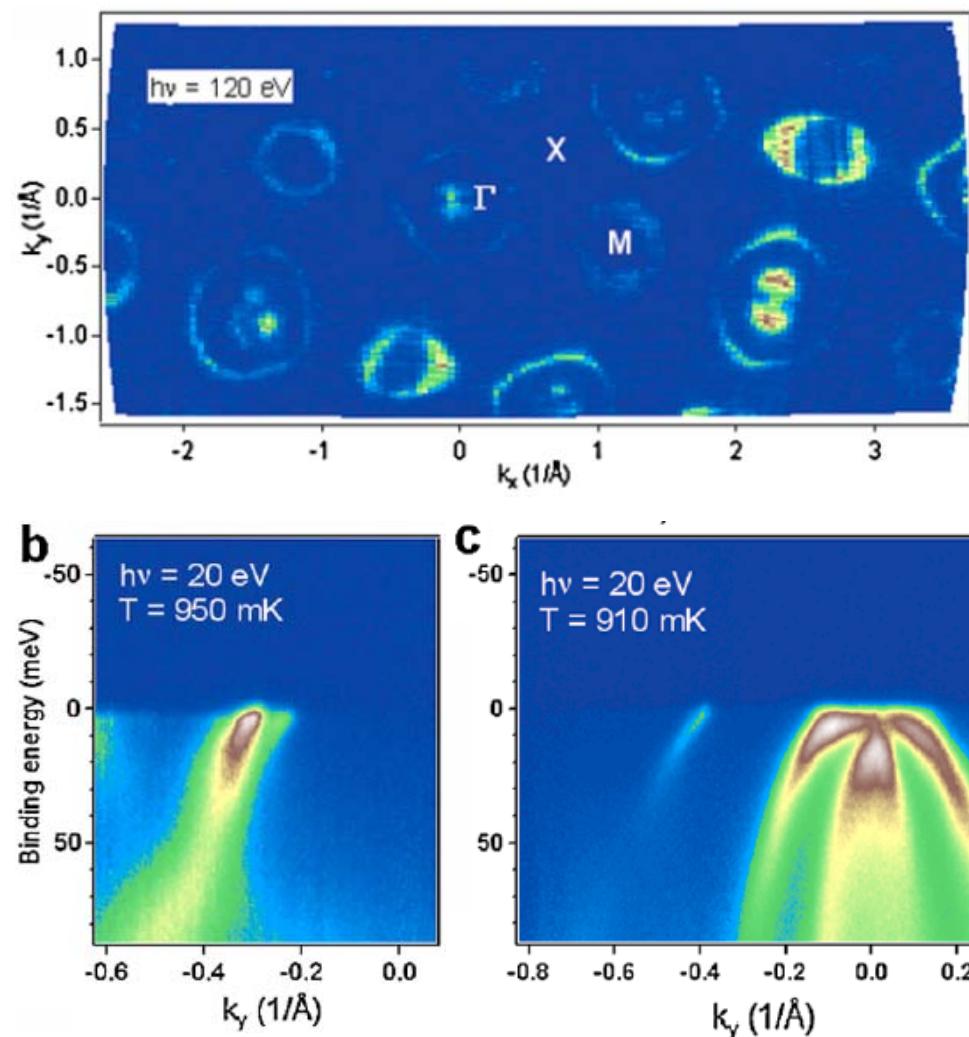
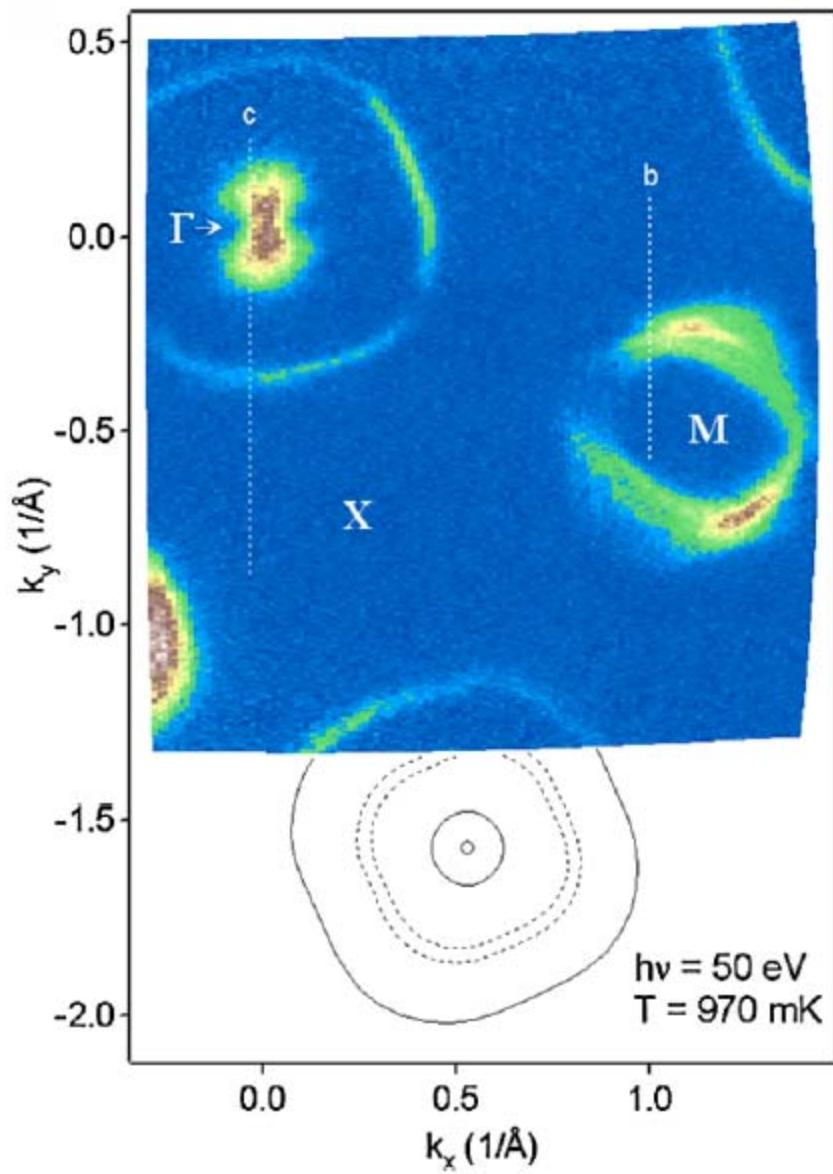


Perfectly ARPESable LiFeAs

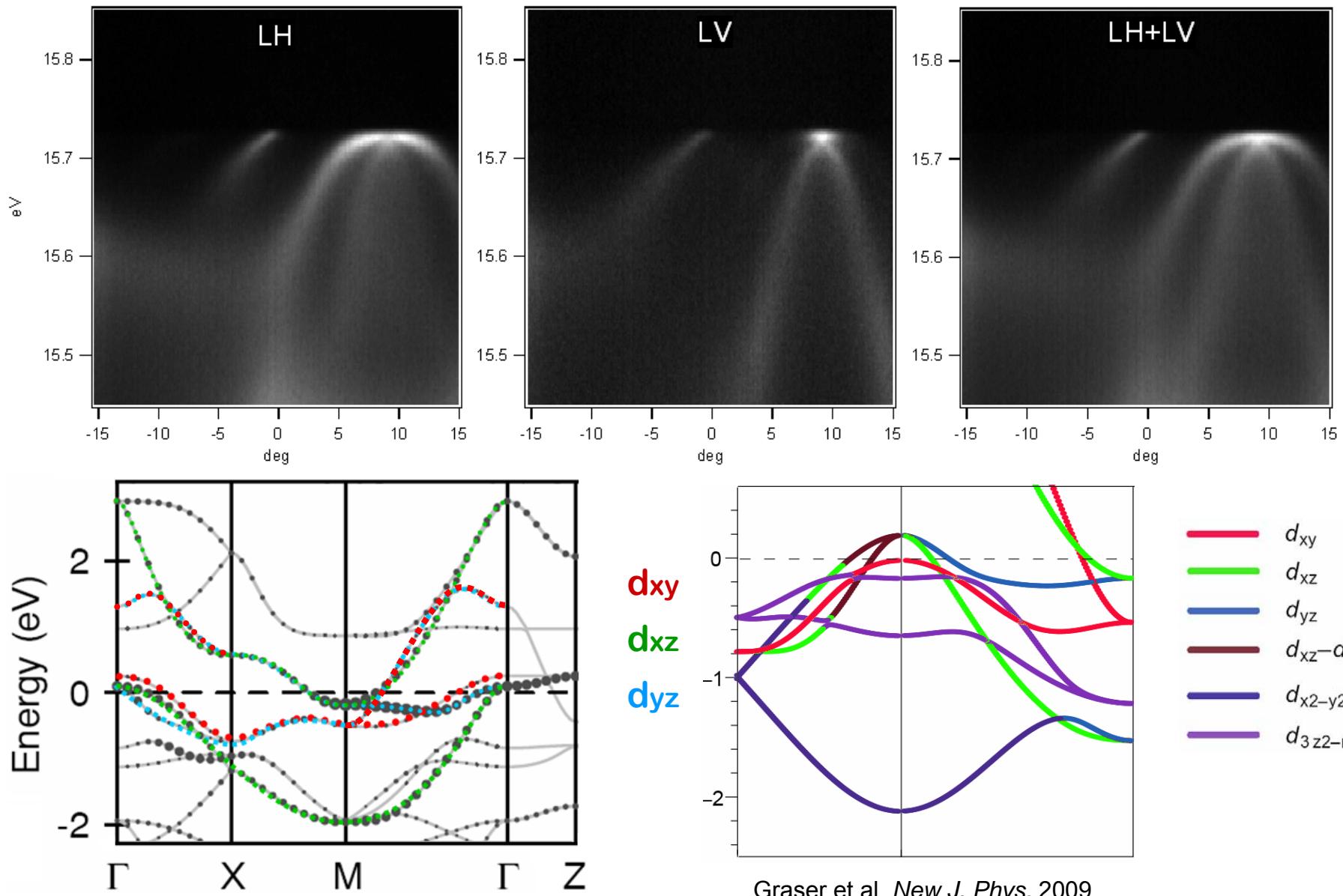


1. Superconducting with $T_c = 18$ K but non-magnetic...
2. Stoichiometric = impurity clean.
3. Perfectly two-dimensional Fe-3d_{xy} band well separated from other bands: easy to analyse its fine structure.
4. Cleaves between the two Li layers => non-polar surface.

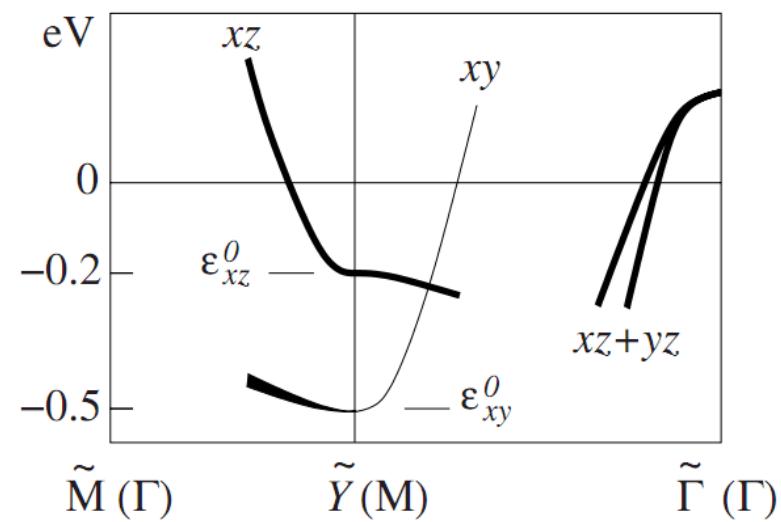
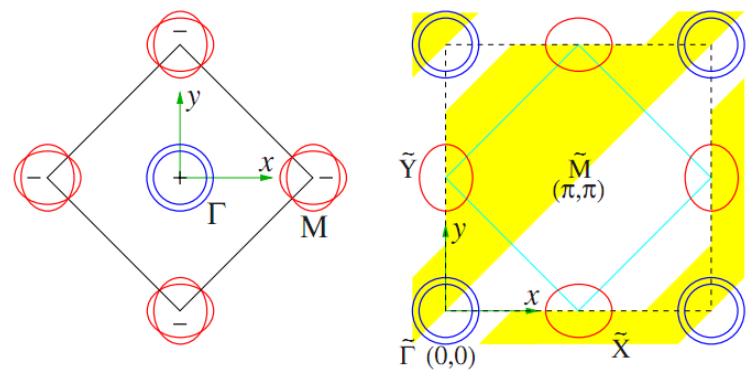
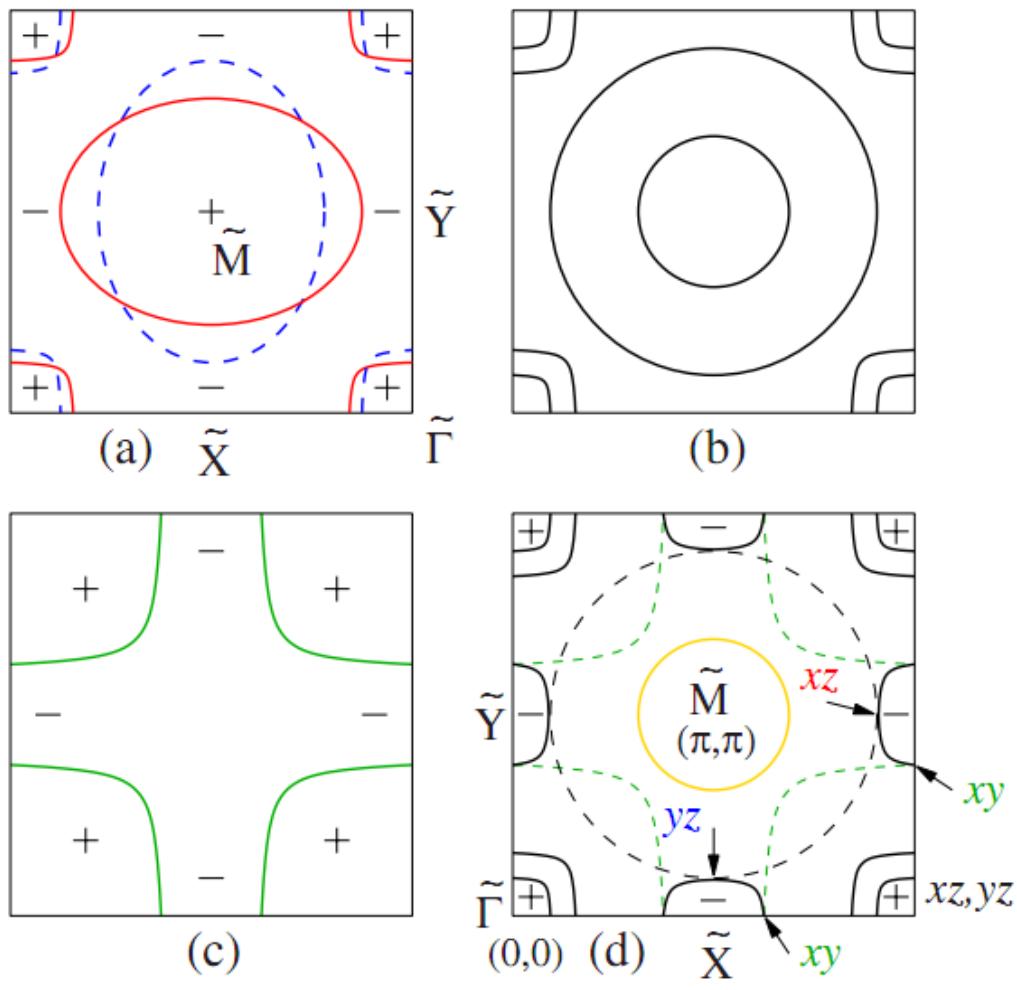
LiFeAs: band structure



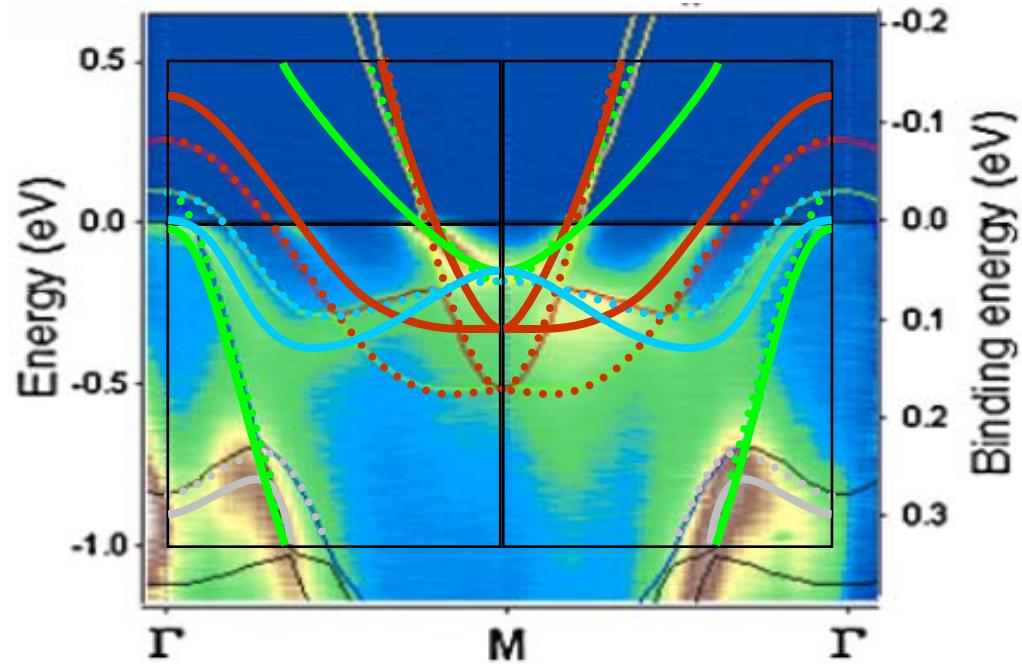
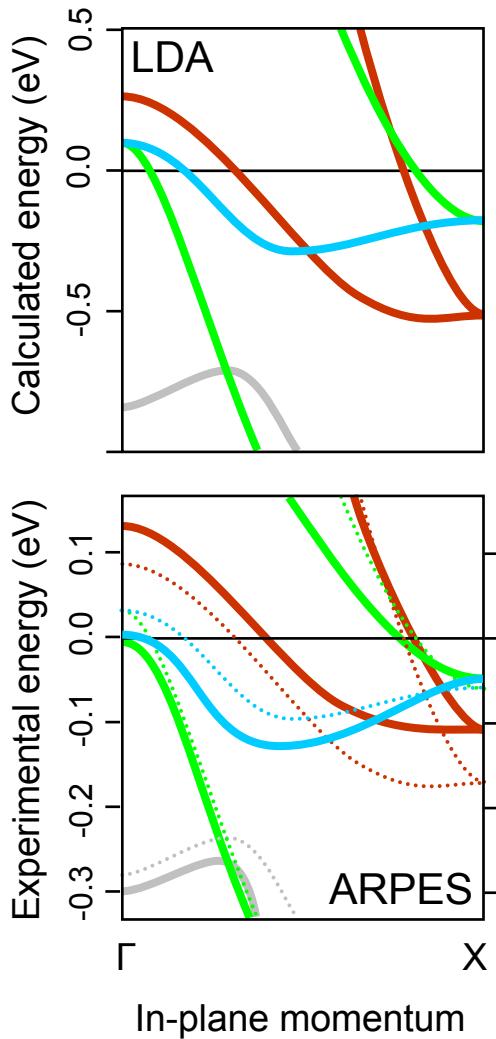
LiFeAs: band structure



Three orbital model

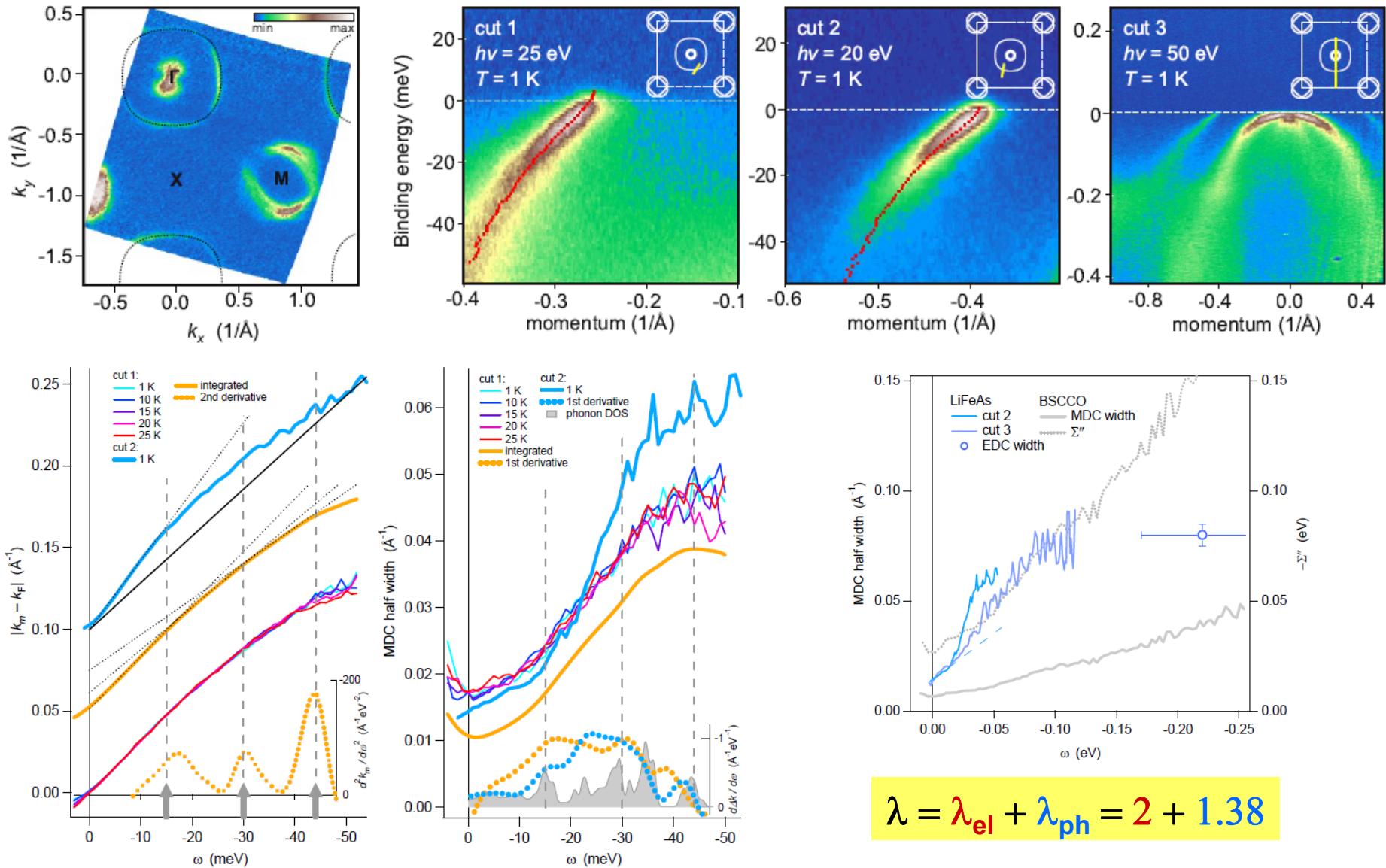


LiFeAs: band structure

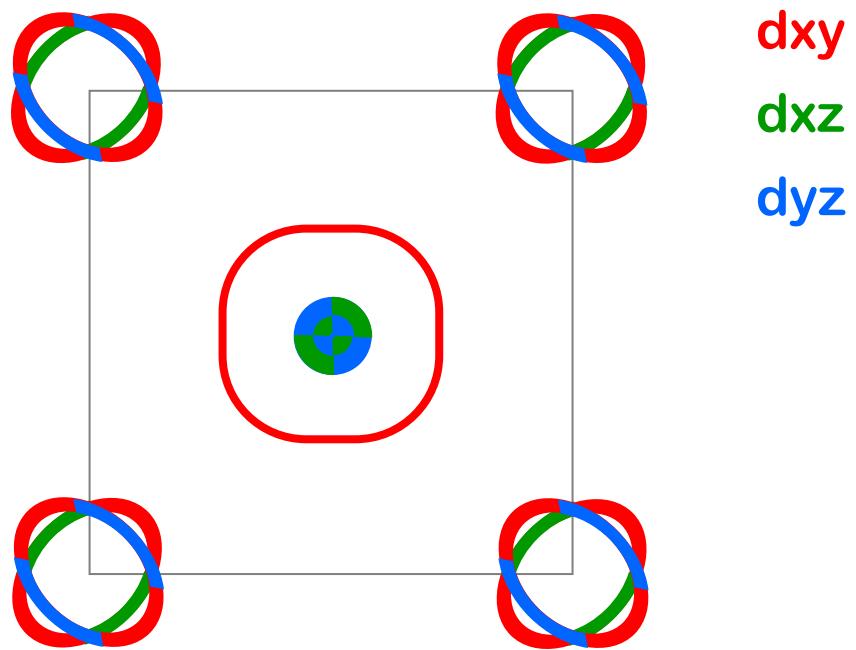
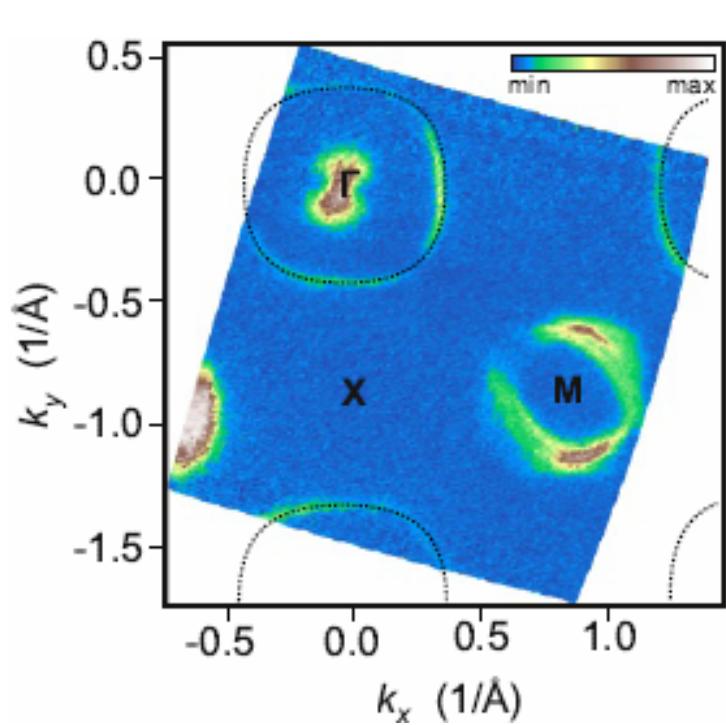


- 3 times renormalized;
- **dxy** band is 60 (**bare 180**) meV higher:
no FS nesting;
- **dxz/dyz** bands are 40 (**120**) meV lower;
- **dxz/dyz** bands are flattened or “pinned”
to the Fermi level.

LiFeAs: renormalization



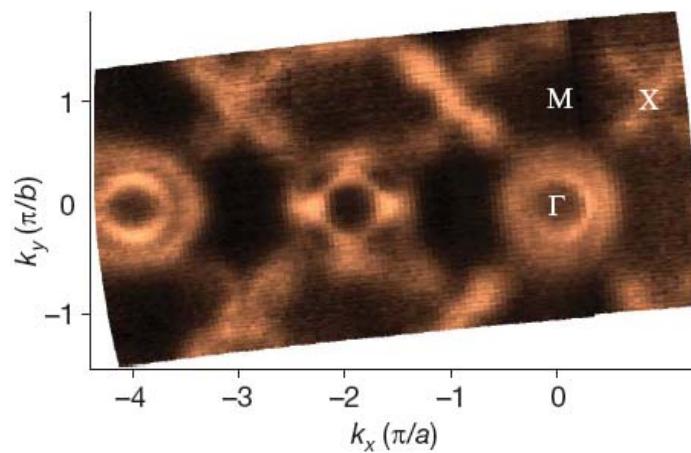
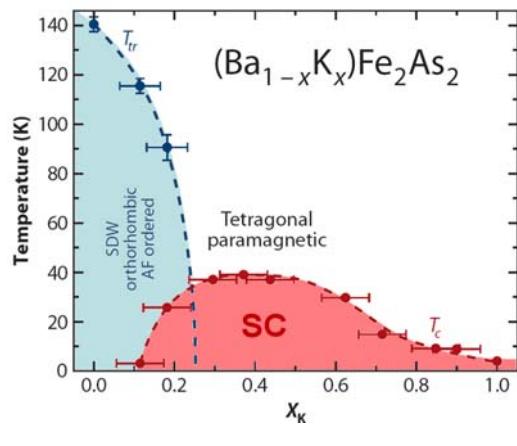
LiFeAs: FS orbital character



122

hole doped

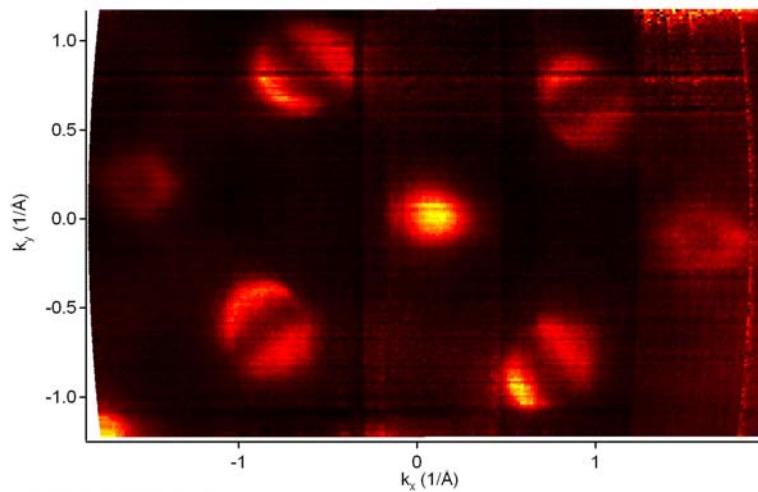
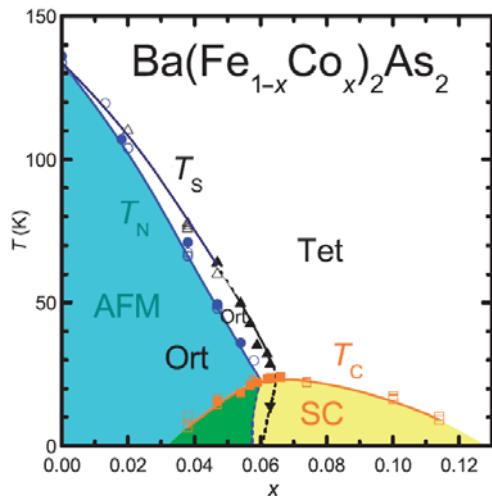
BaFe_2As_2 (BFA) • $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (BKFA) • KFA
 $\text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$ (BNFA)



122

electron doped

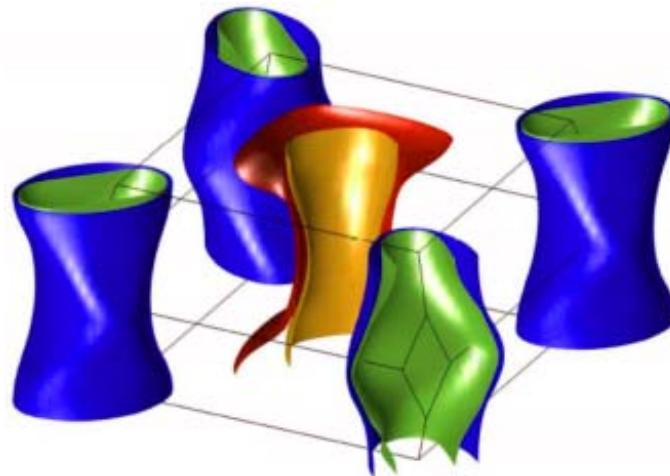
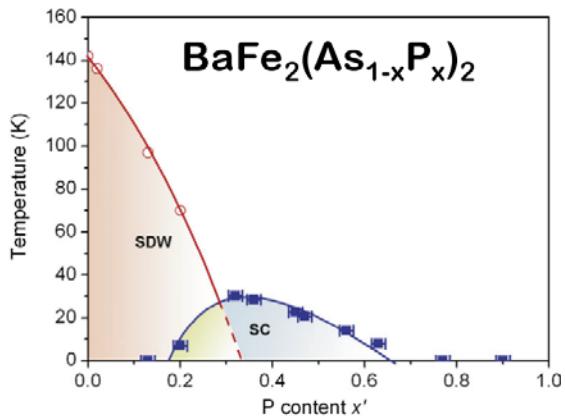
BFA • $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (BFCA)



122

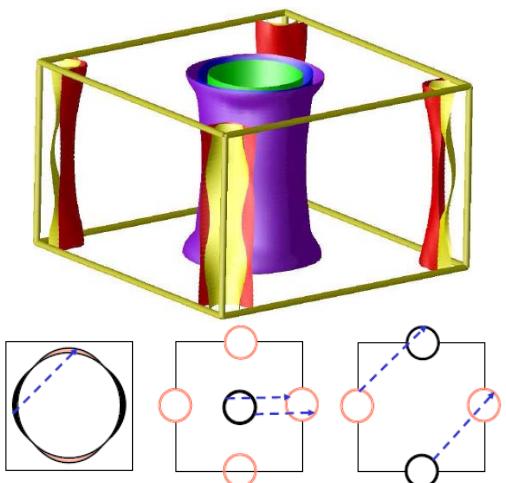
isovalent doping

$\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ (BFAP)

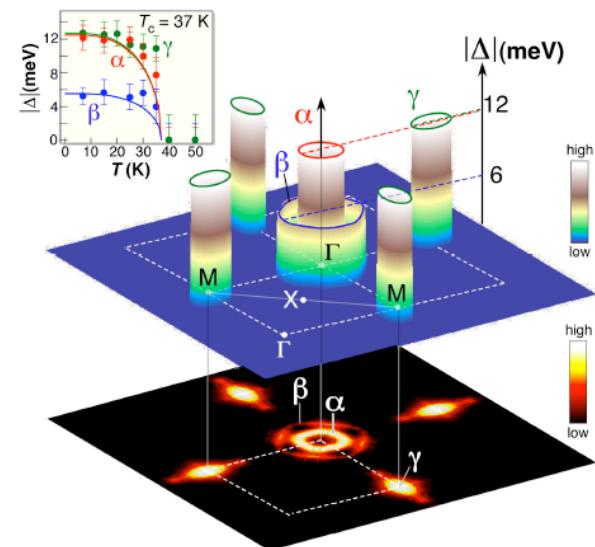
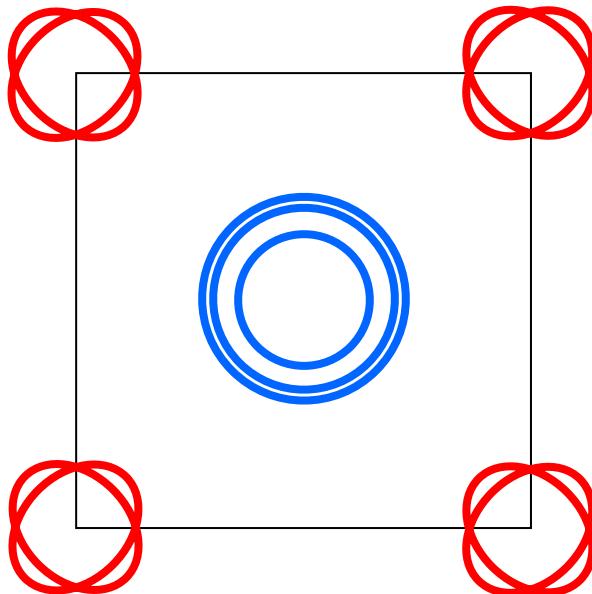


H. Shishido et al. PRL 2010

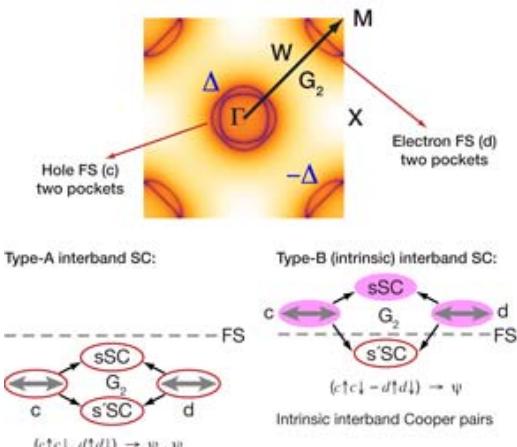
Fermi surface of BKFA



Mazin & Schmalian 2009

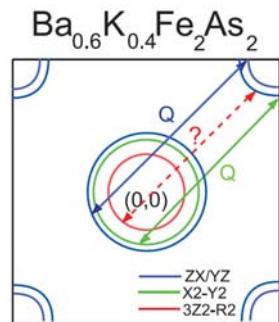


Ding EPL 2008

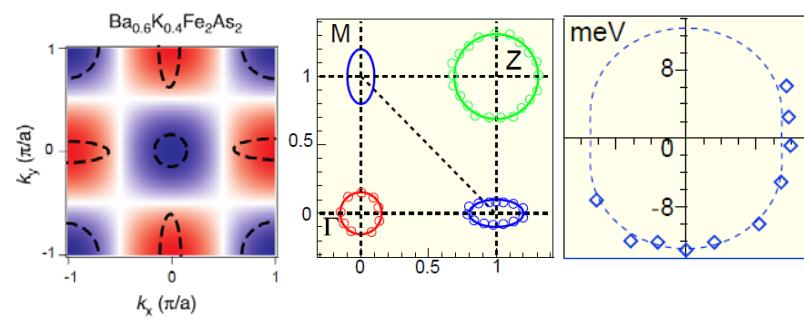


Intraband Cooper pairing
further enhanced by G_2

Tesanovic Physics 2009

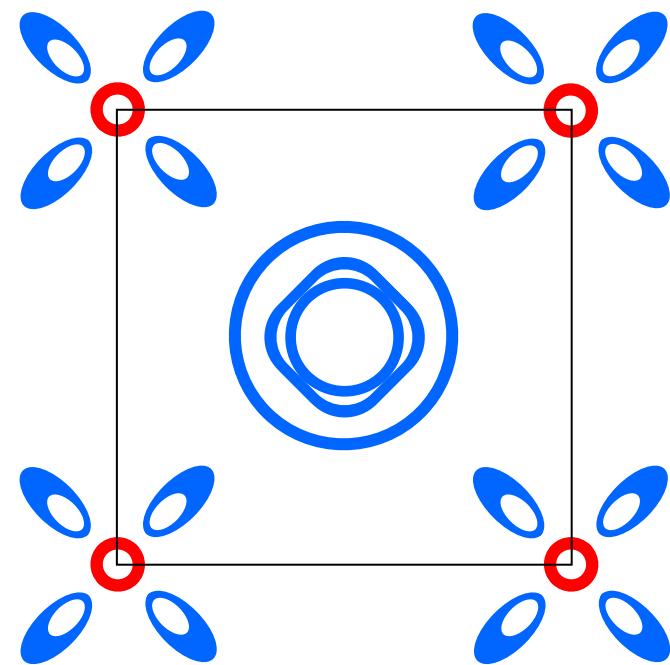
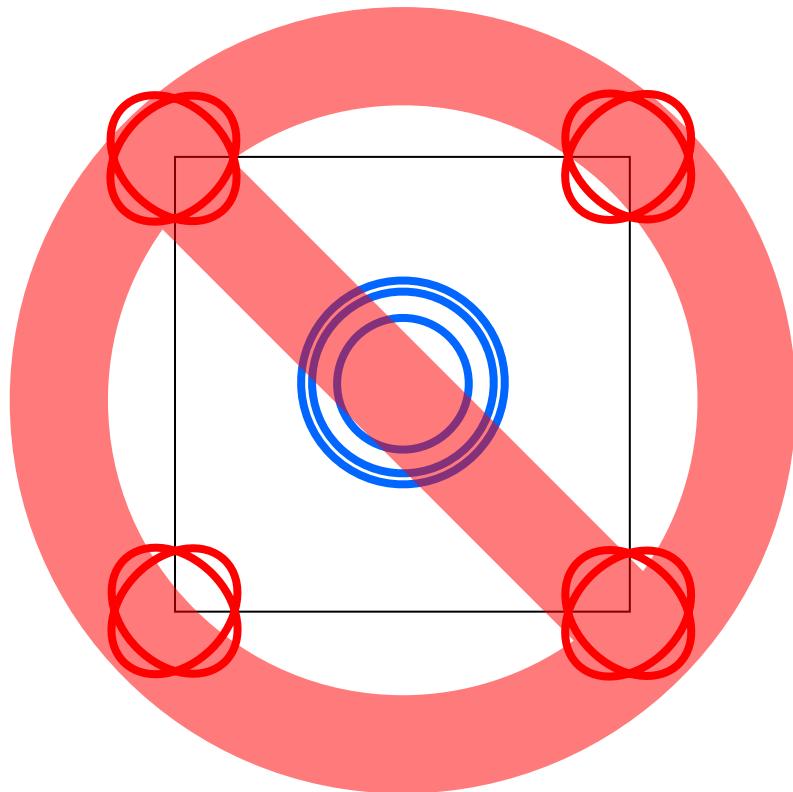


Shimojima Science 2011

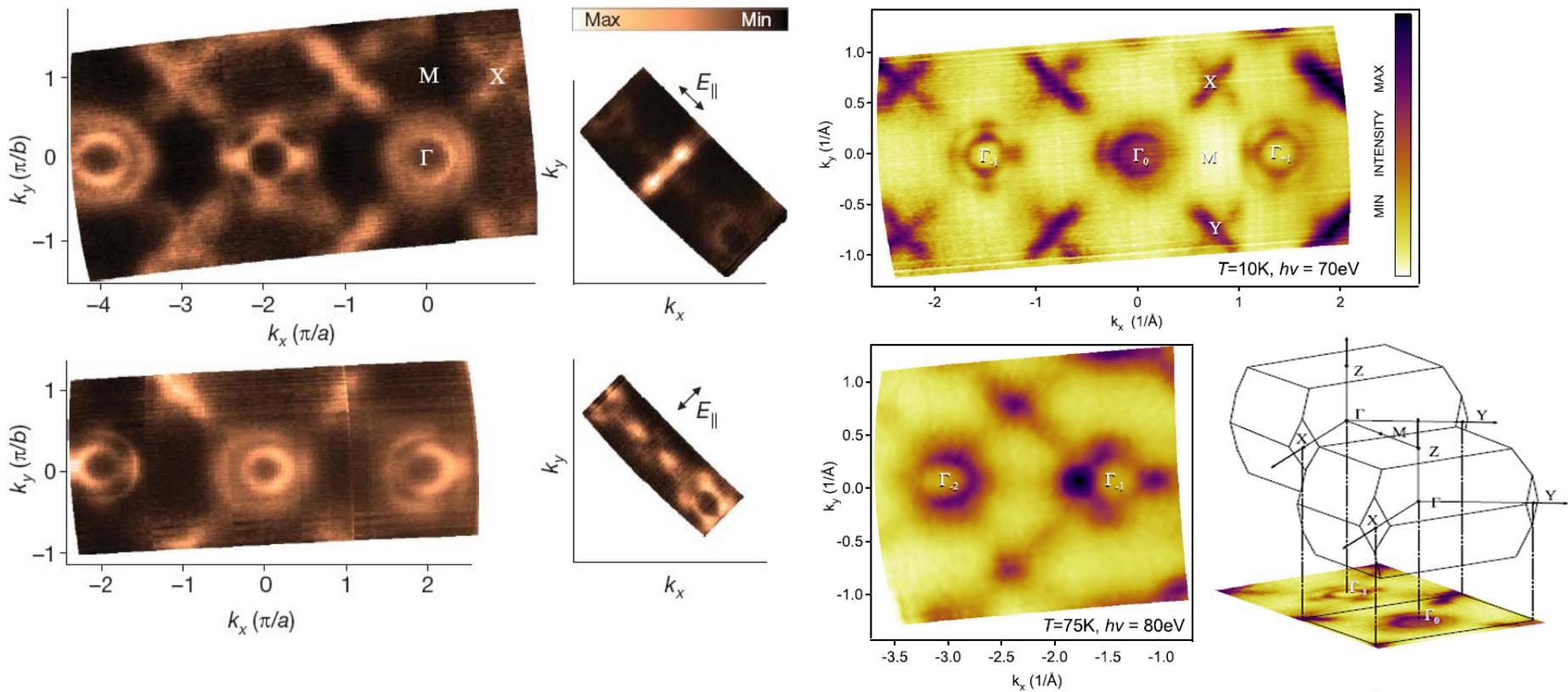


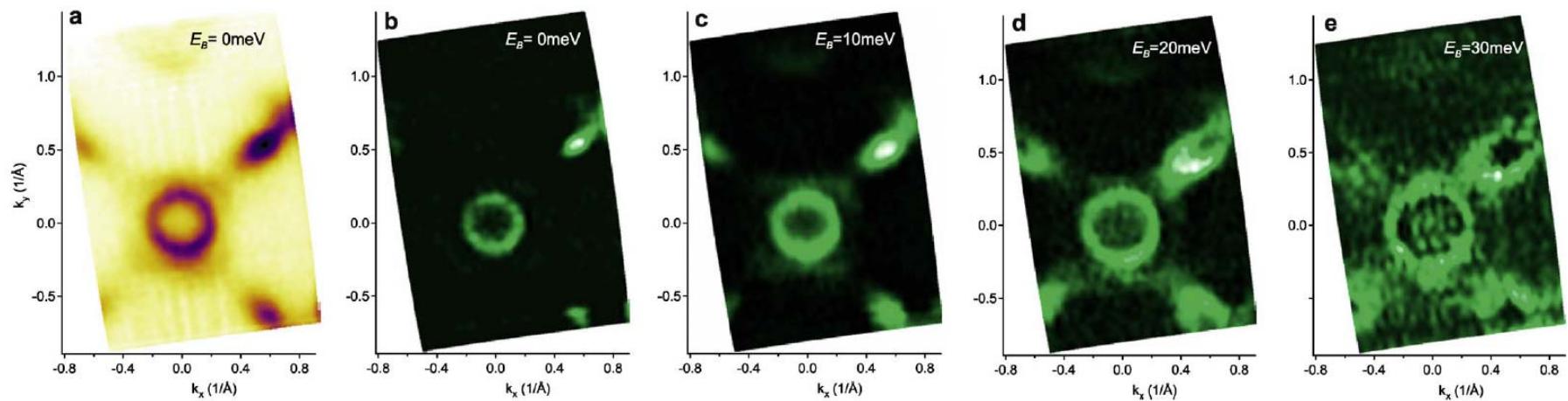
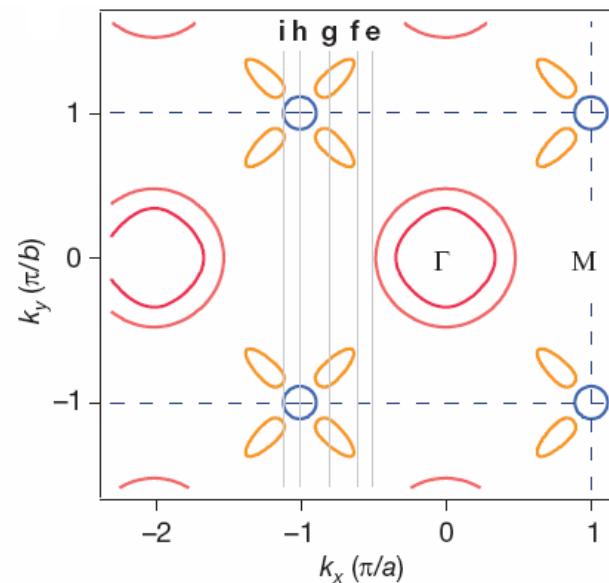
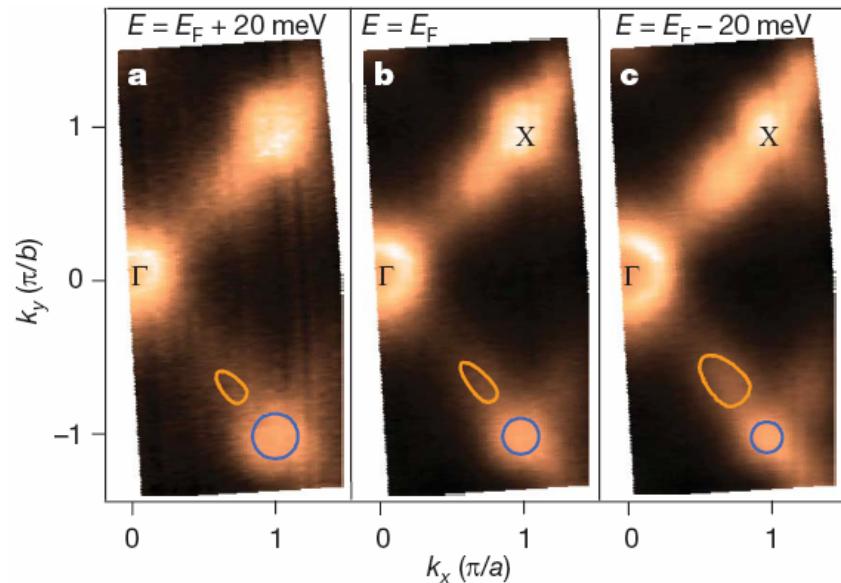
Hu & Ding arXiv:1107.1334

Fermi surface of BKFA



Fermi surface of BKFA

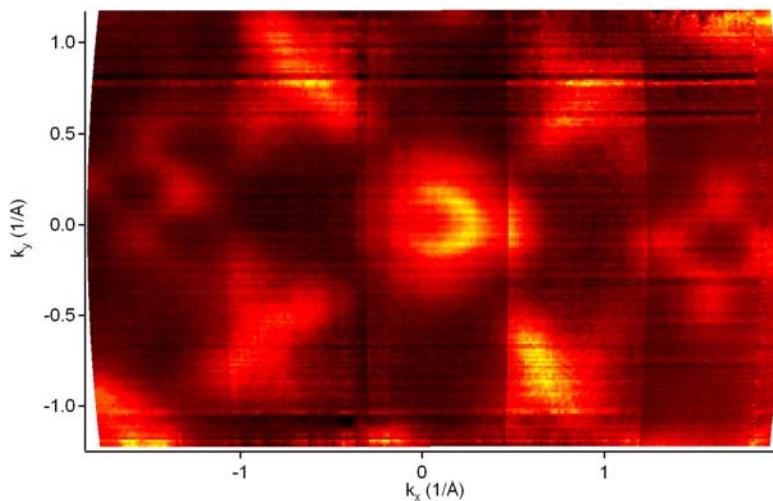




Propeller FS in 122

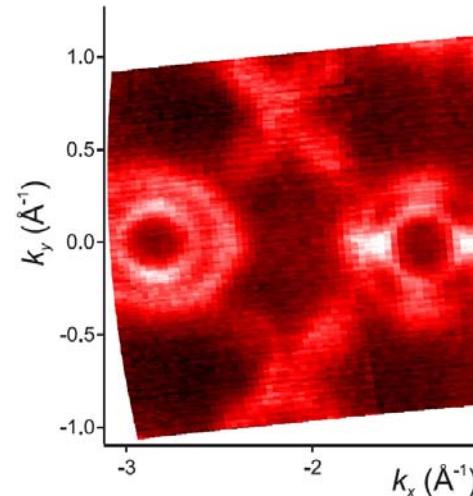
$\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

$\omega = -90 \text{ meV}, h\nu = 80 \text{ eV}$



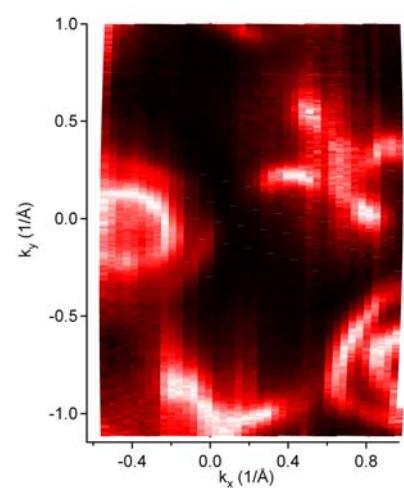
$\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$

$\omega = 0, h\nu = 80 \text{ eV}$



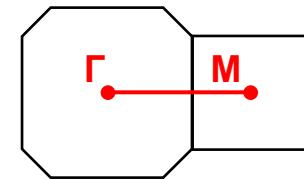
$\text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$

$\omega = 0, h\nu = 80 \text{ eV}$

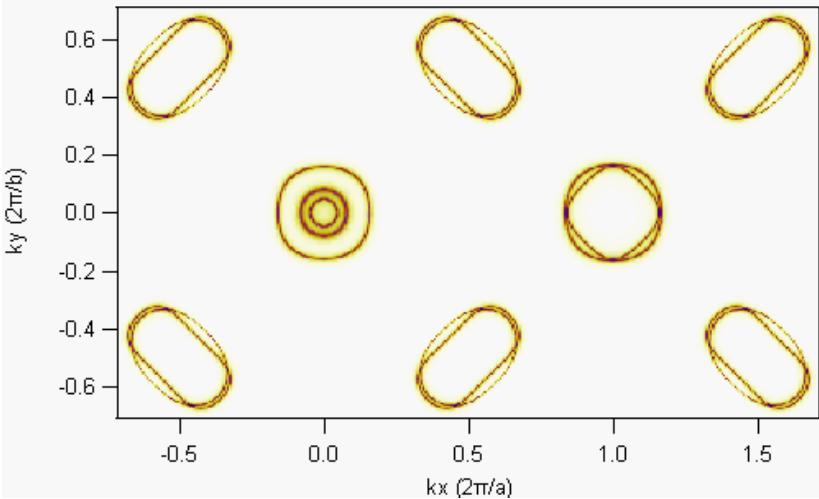


Evtushinsky 2010

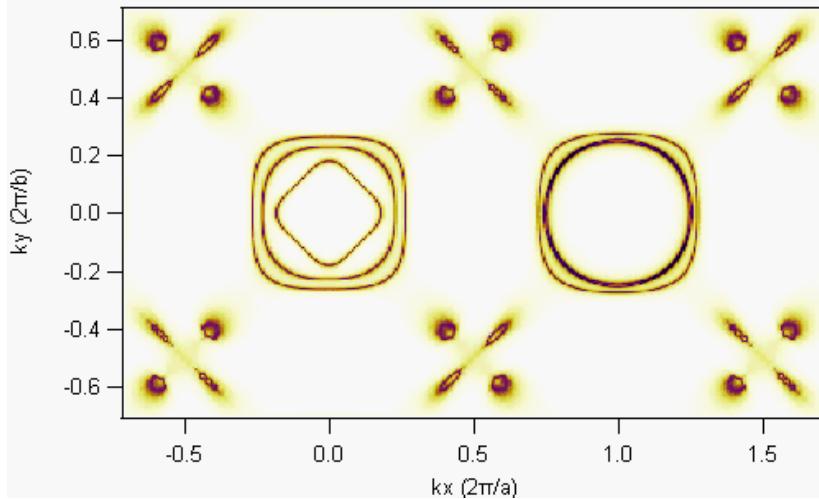
Calculated FC of BFA - BKFA



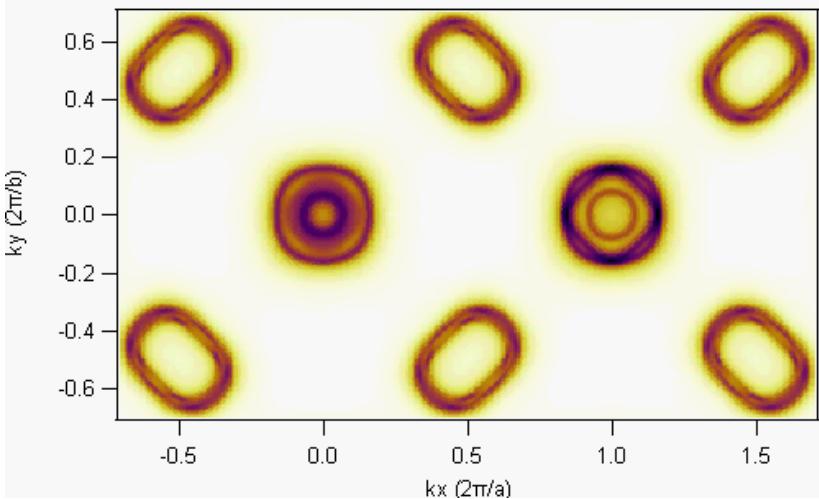
$z = 0.000 \quad dz = 0.000 \quad Ef = 0.000$



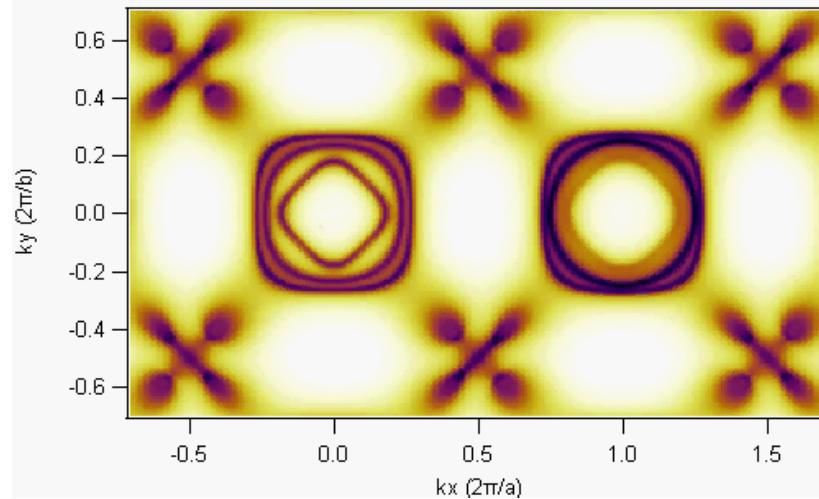
$z = 0.000 \quad dz = 0.000 \quad Ef = 0.076$



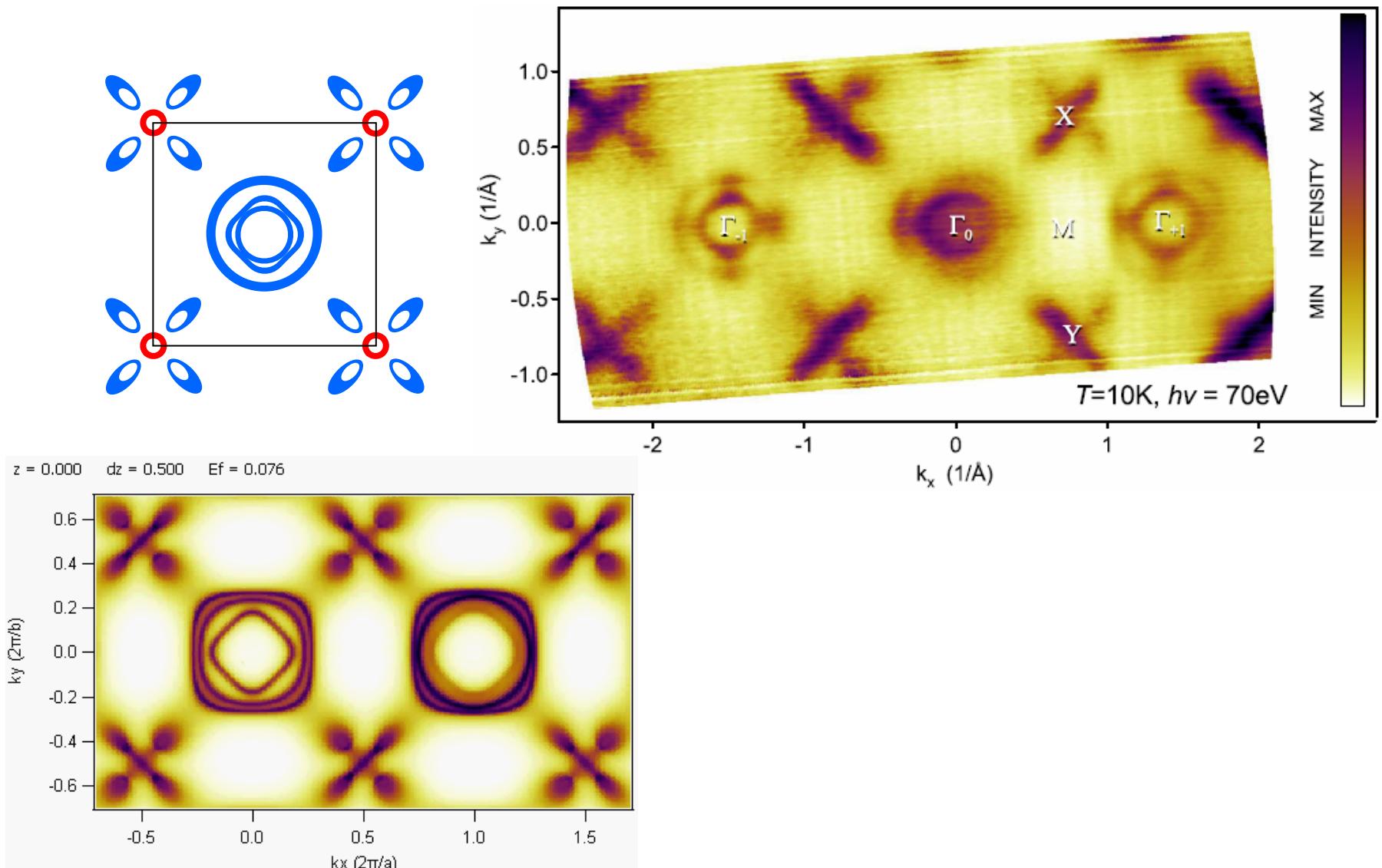
$z = 0.000 \quad dz = 0.500 \quad Ef = 0.000$



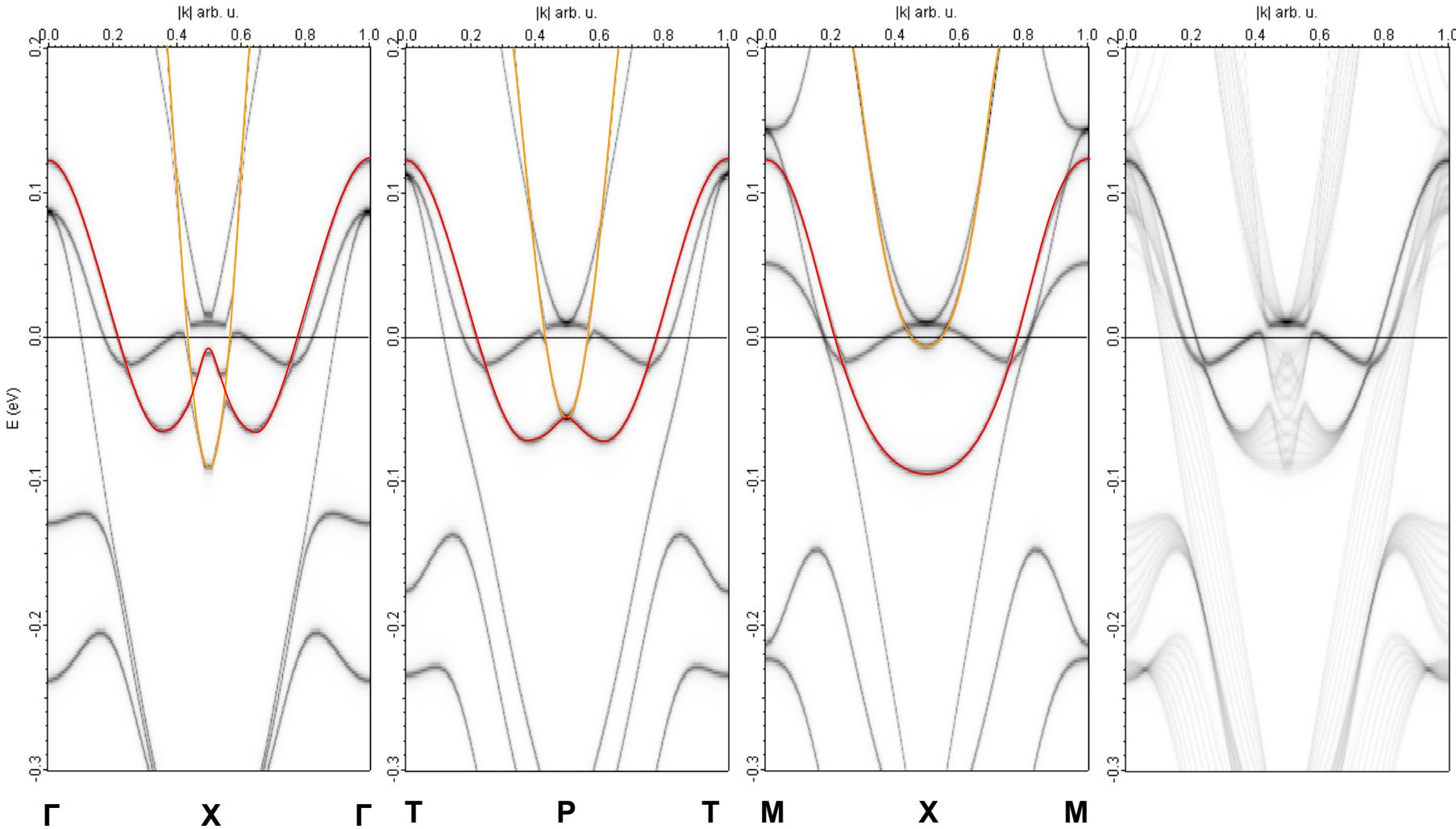
$z = 0.000 \quad dz = 0.500 \quad Ef = 0.076$

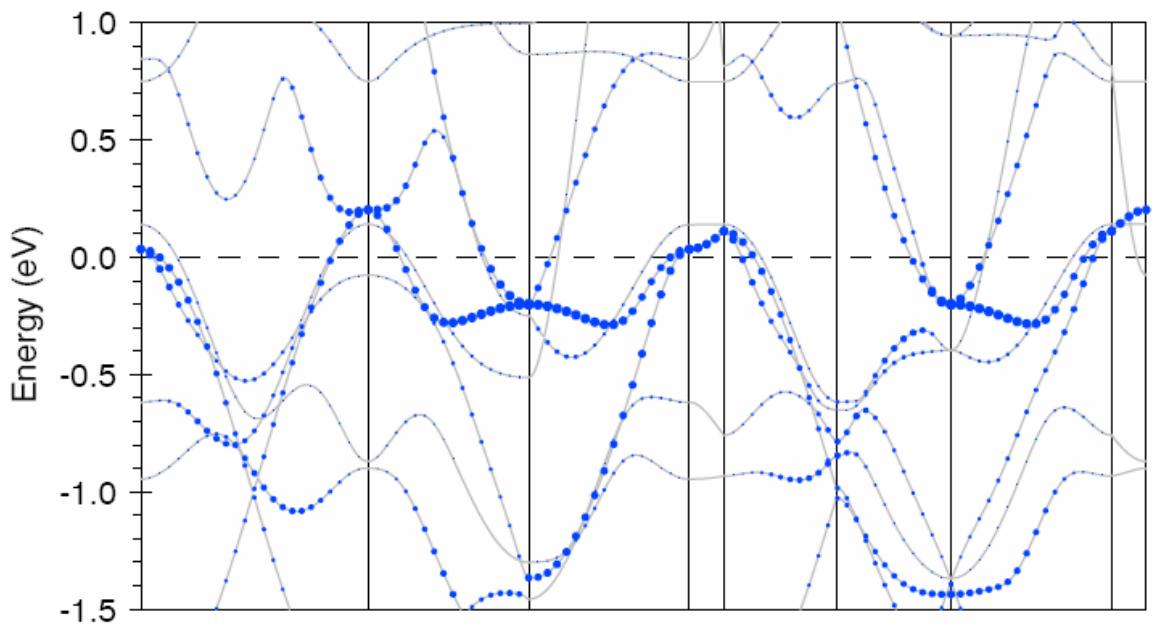


BKFA: exp & calc

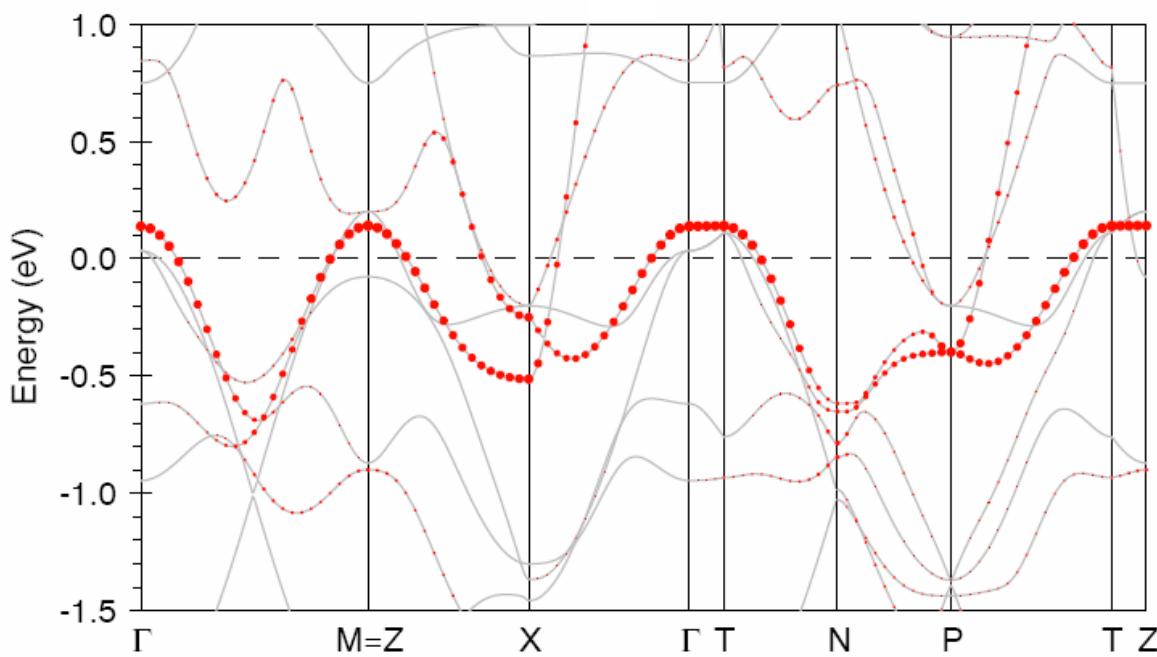


Calculated BFA band structure renormalized and shifted by 76 meV



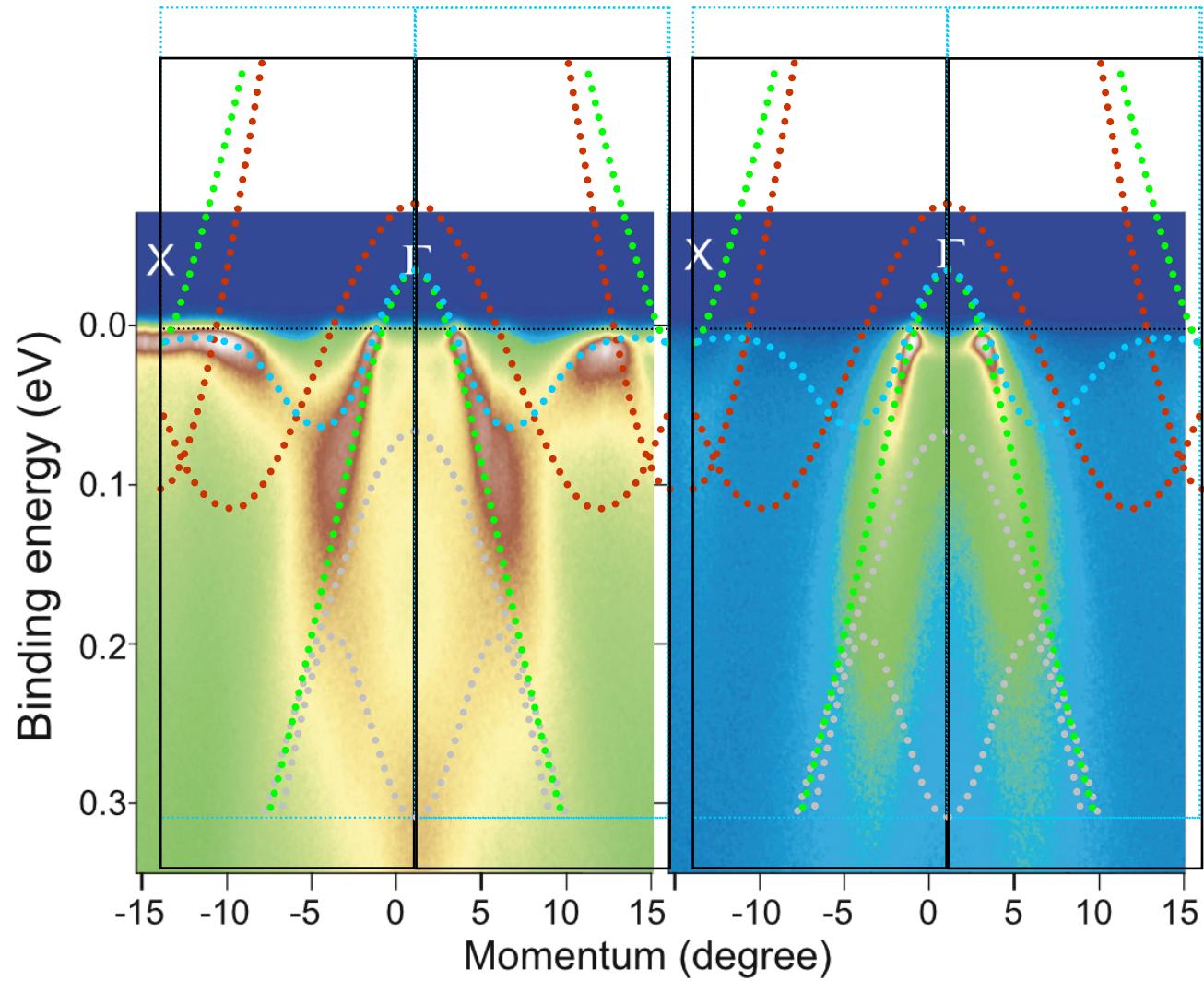
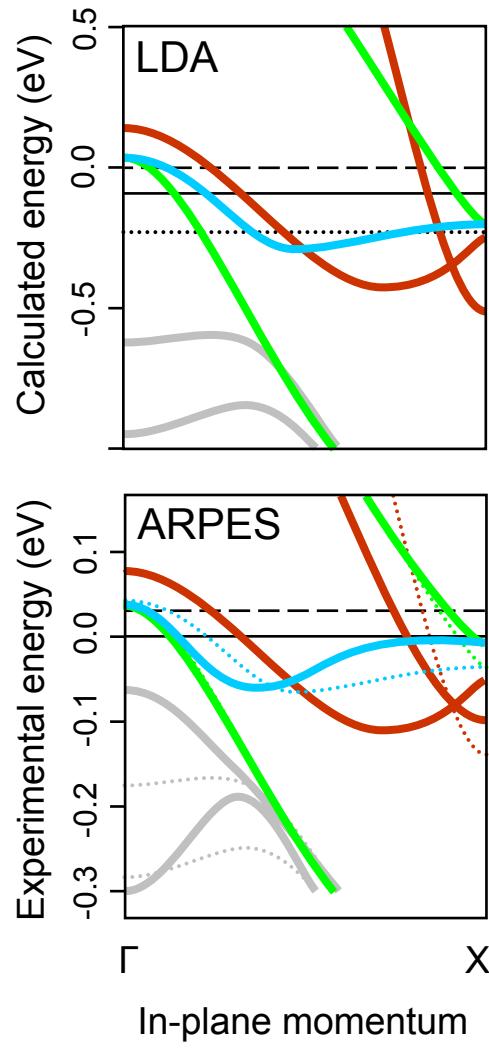


$d_{xz} + d_{yz}$

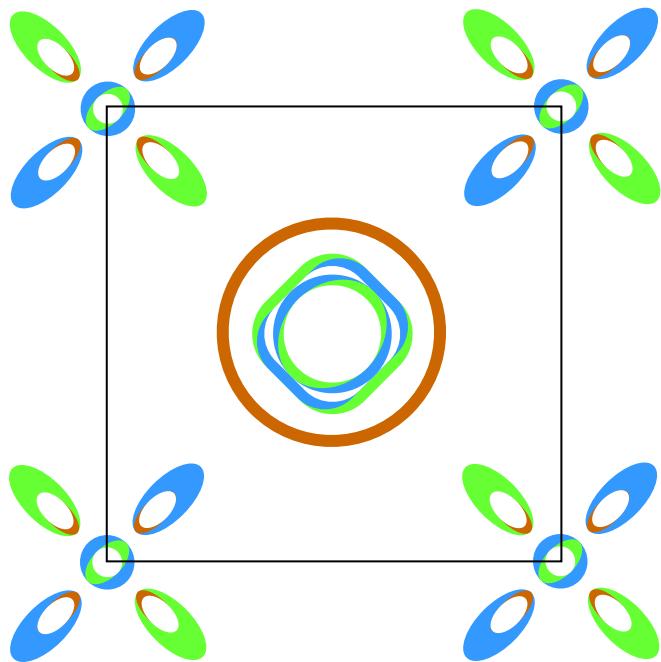


d_{xy}

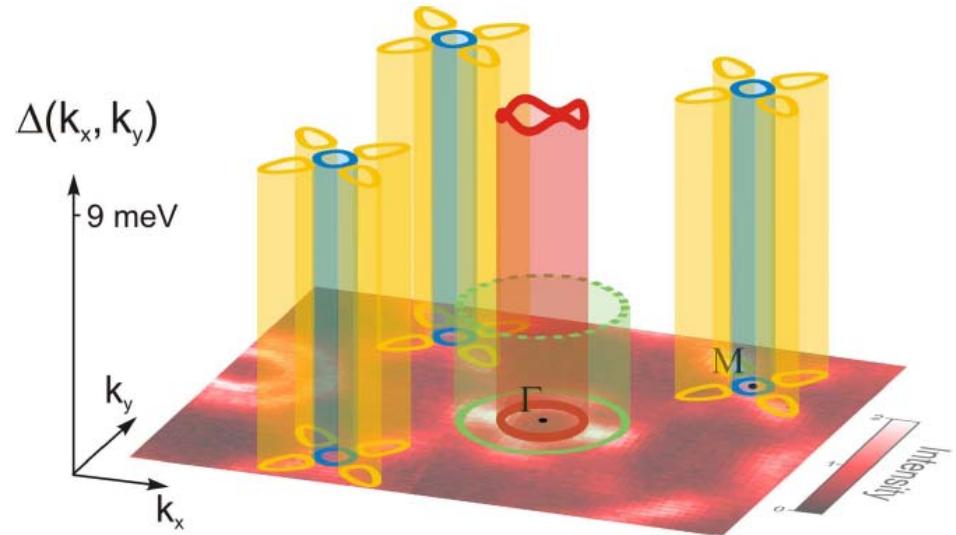
BKFA: band structure



BKFA: Fermi surface and gaps



d_{xy}
 d_{xz}
 d_{yz}

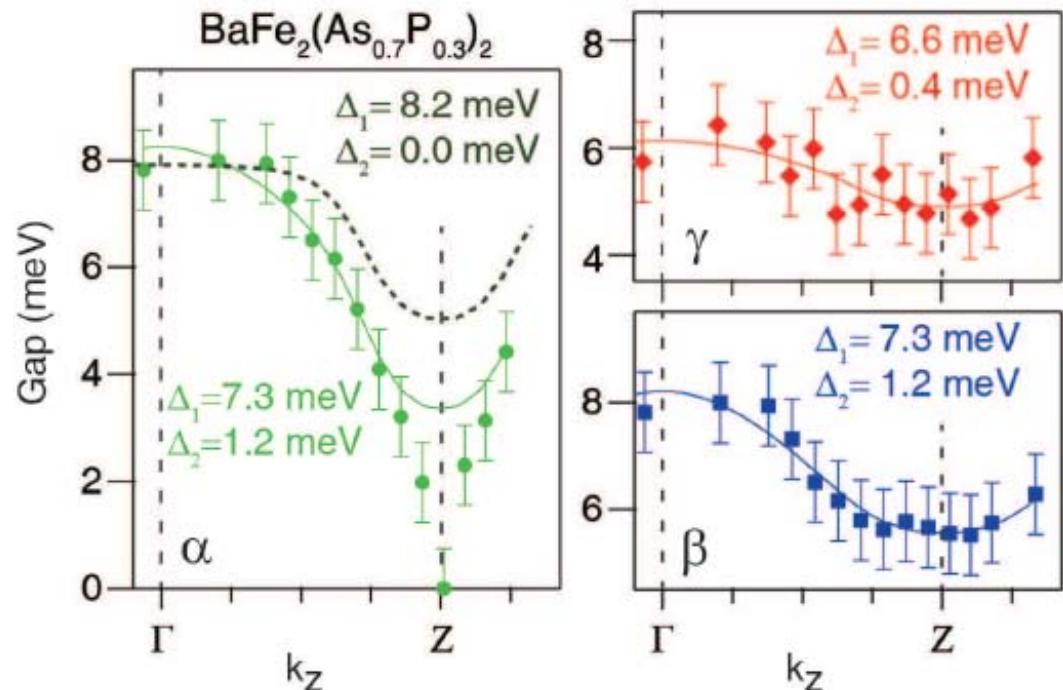
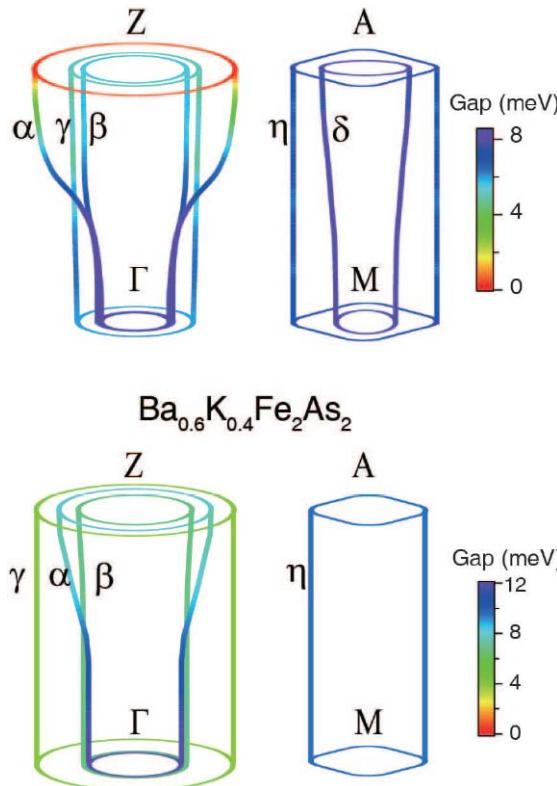
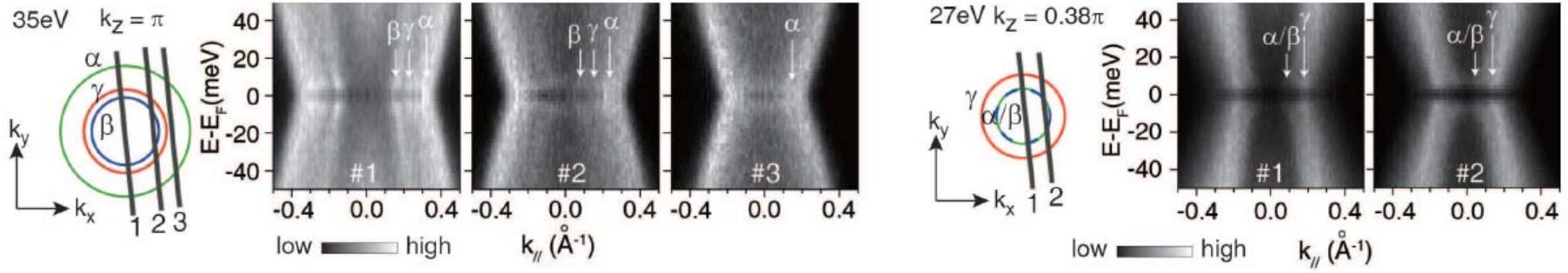


D. Evtushinsky [PRB 2009](#), [NJP 2009](#)

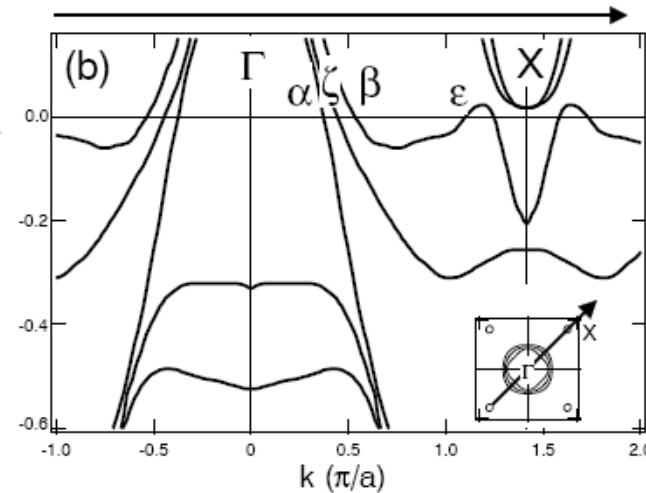
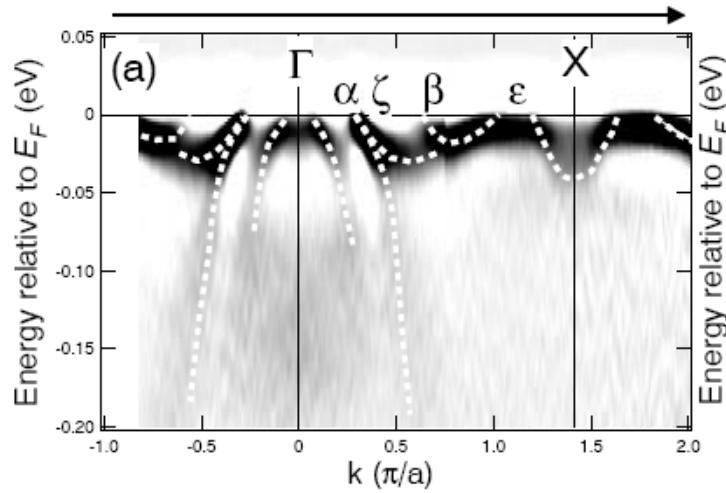
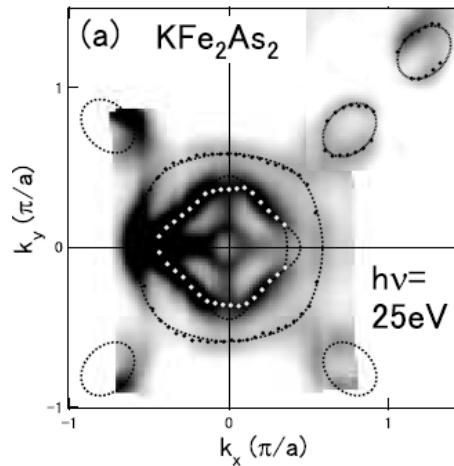
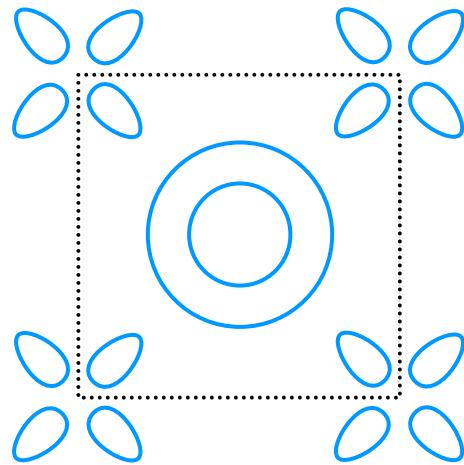
Δ correlates with the orbital composition:
 $\Delta = 3\text{--}4 \text{ meV}$ for $3d_{xy}$ and $3d_{z^2}$
 $\Delta = 10.5 \text{ meV}$ for $3d_{xz}/yz$.

D. Evtushinsky 2011

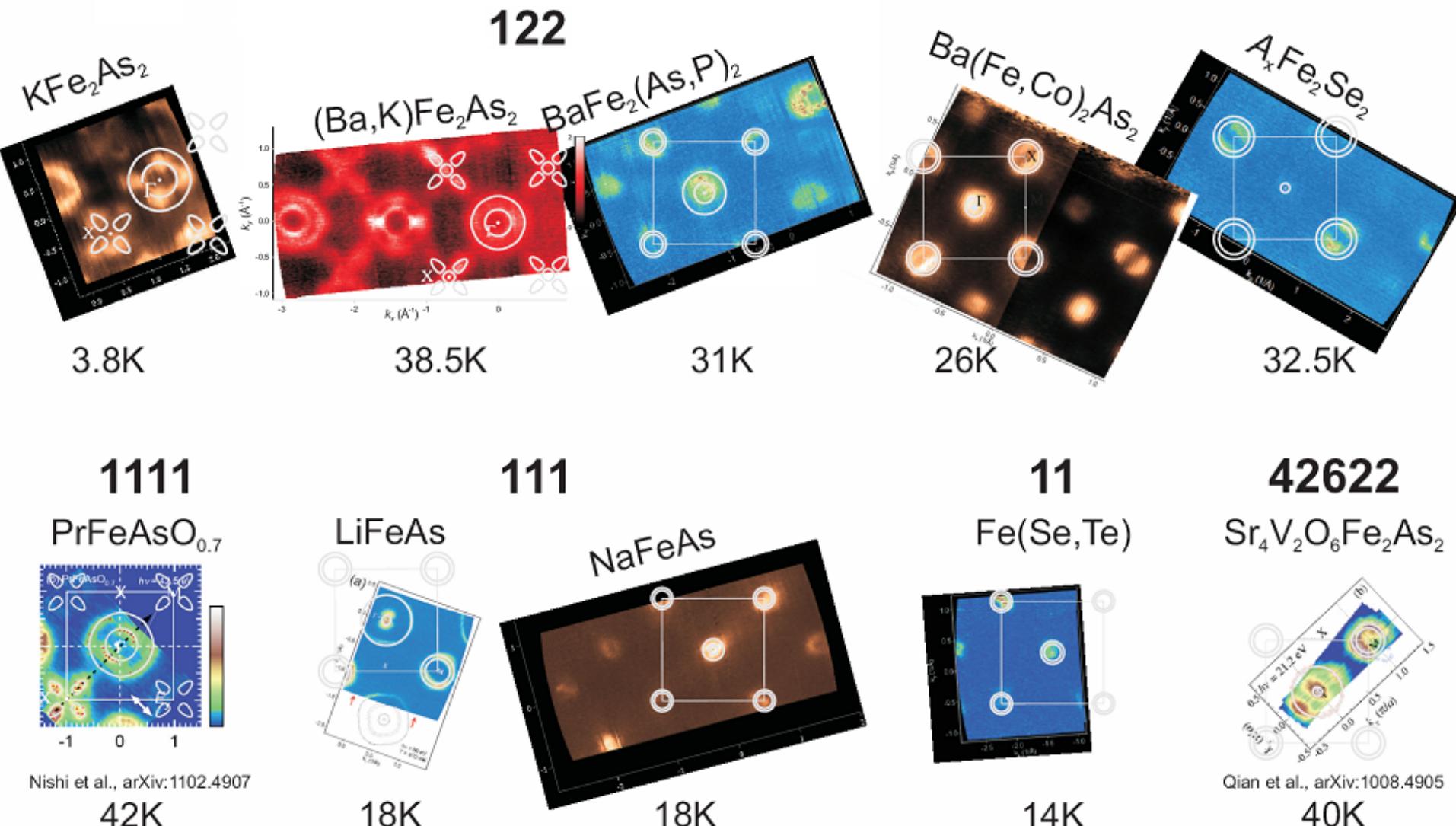
BFAP: node or small gap?



KFA: hole-like Fermi surfaces



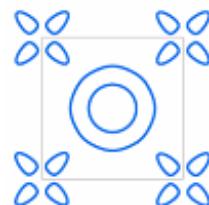
FS's of iron-based superconductors



FS's of iron-based superconductors

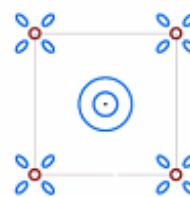
122

KFe_2As_2



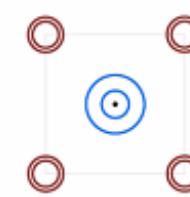
3.8K

$(Ba,K)Fe_2As_2$



38K

$BaFe_2(As,P)_2$



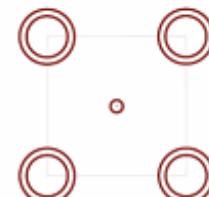
31K

$Ba(Fe,Co)_2As_2$



26K

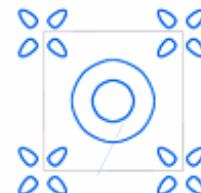
$A_xFe_2Se_2$



31K

1111

$PrFeAsO_{0.7}$



42K

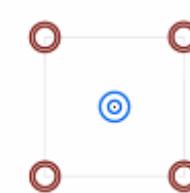
111

$LiFeAs$



18K

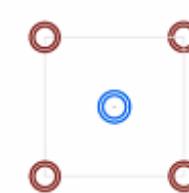
$NaFeAs$



18K

11

$Fe(Se,Te)$



14K

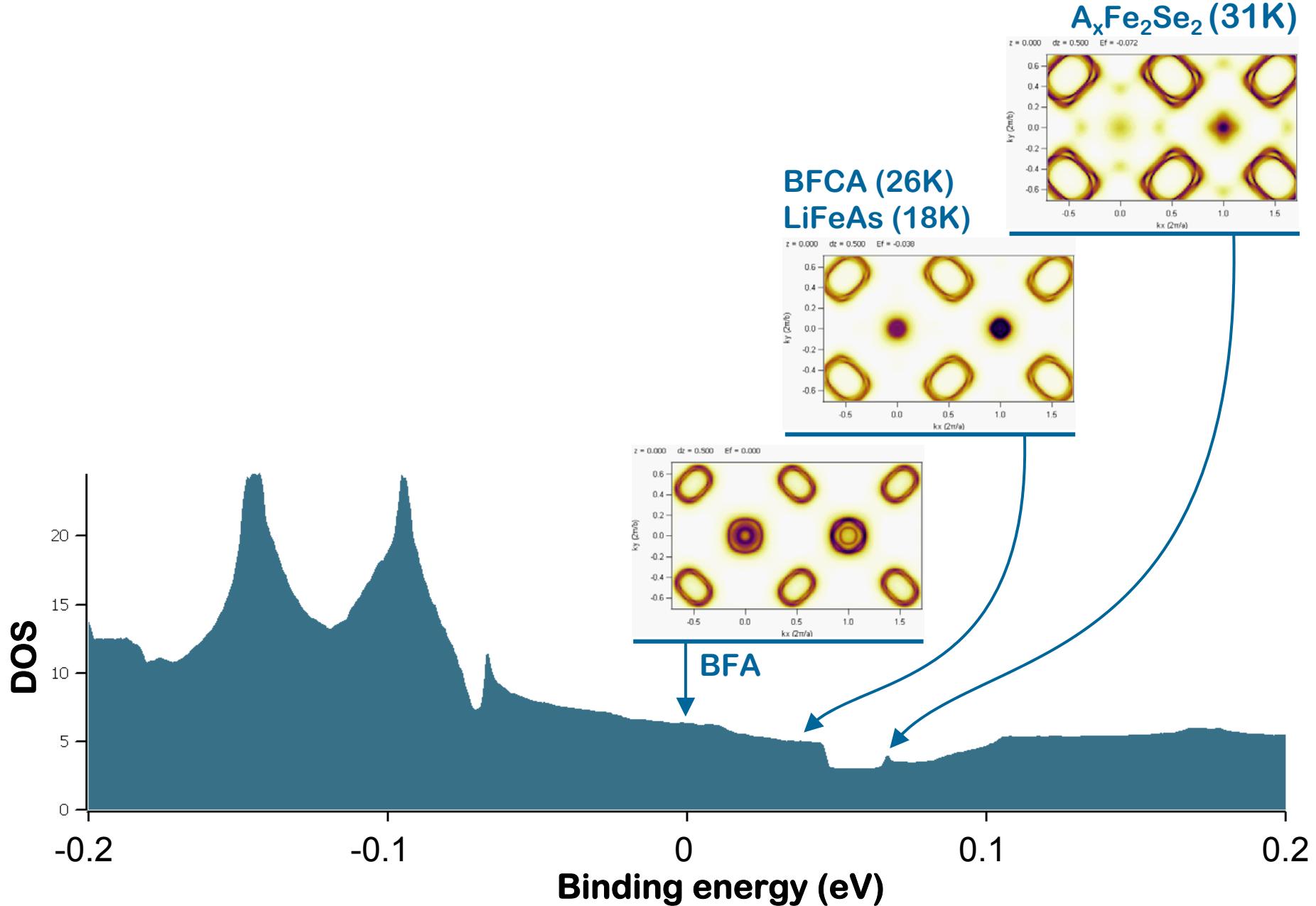
42622

$Sr_4V_2O_6Fe_2As_2$

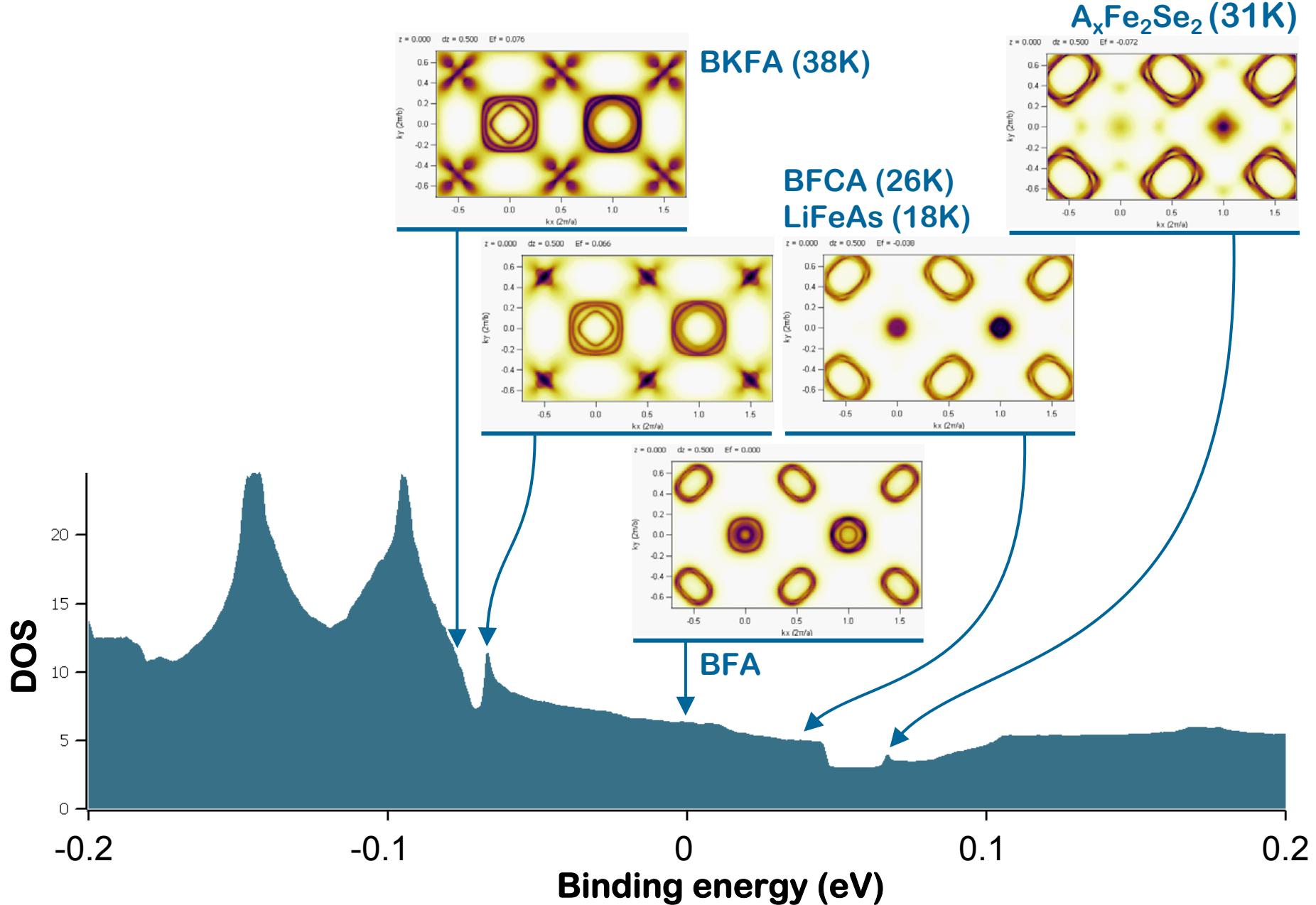


40K

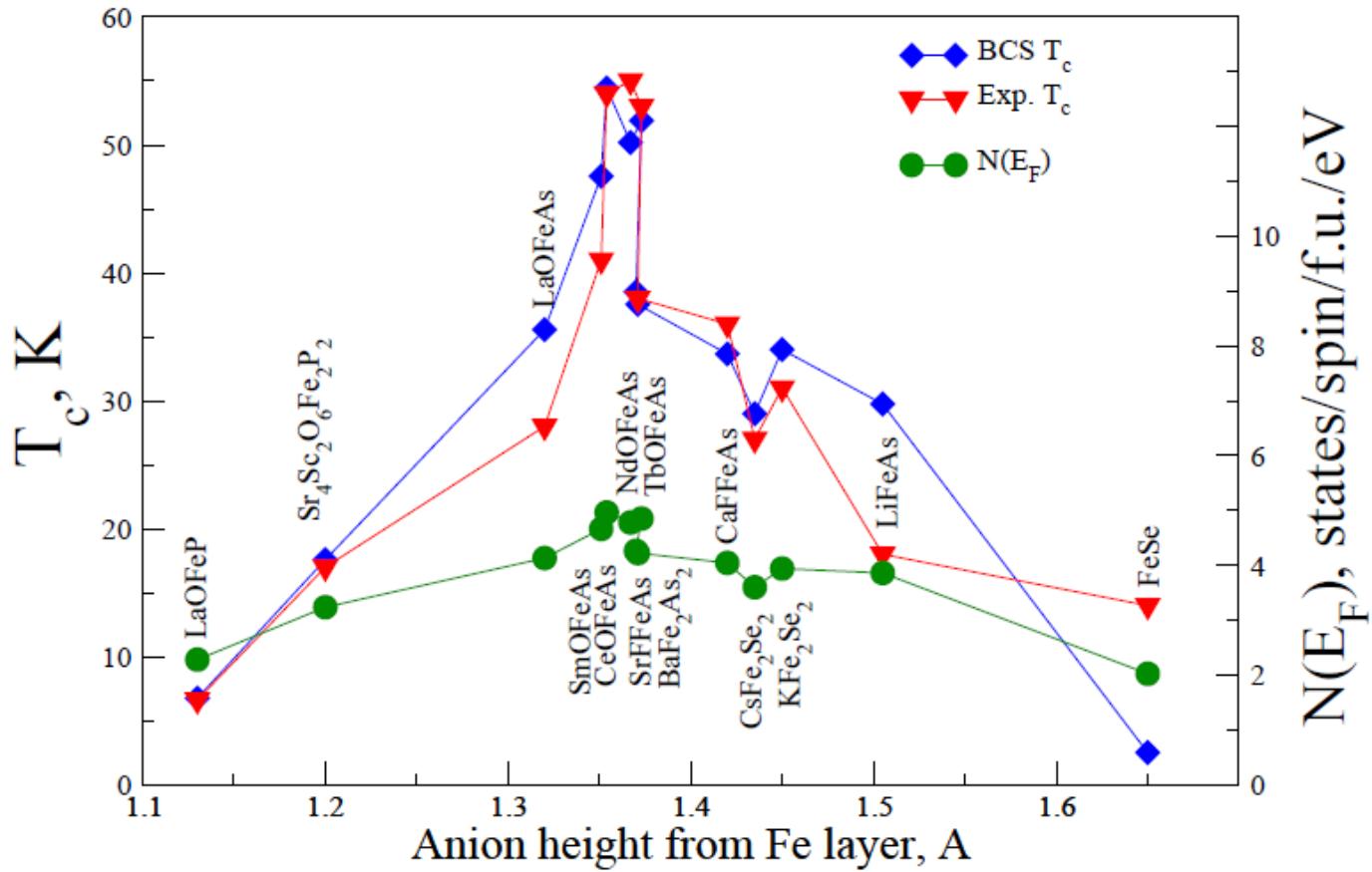
BFA: density of states



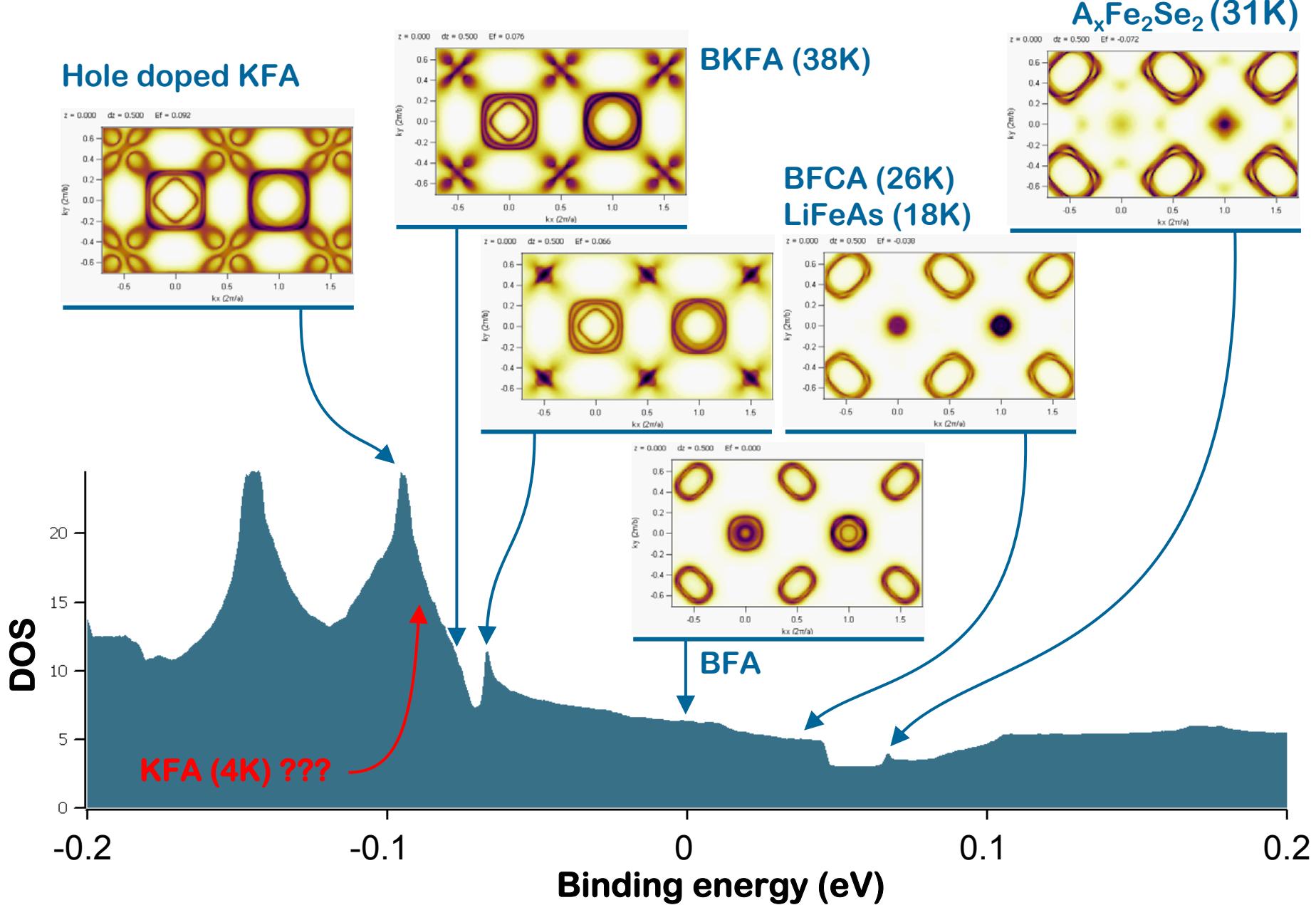
BFA: density of states



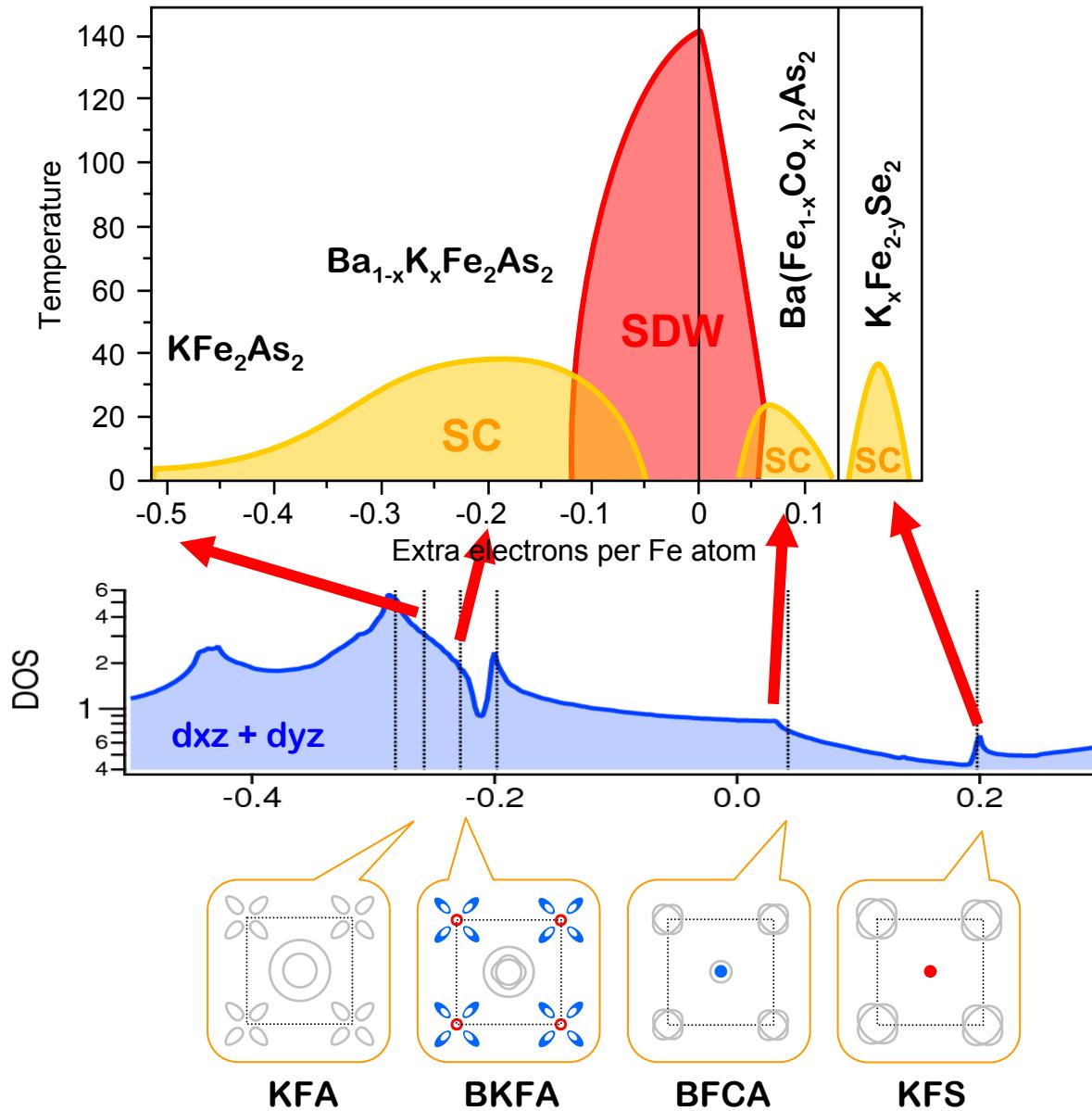
T_c (density of states)?



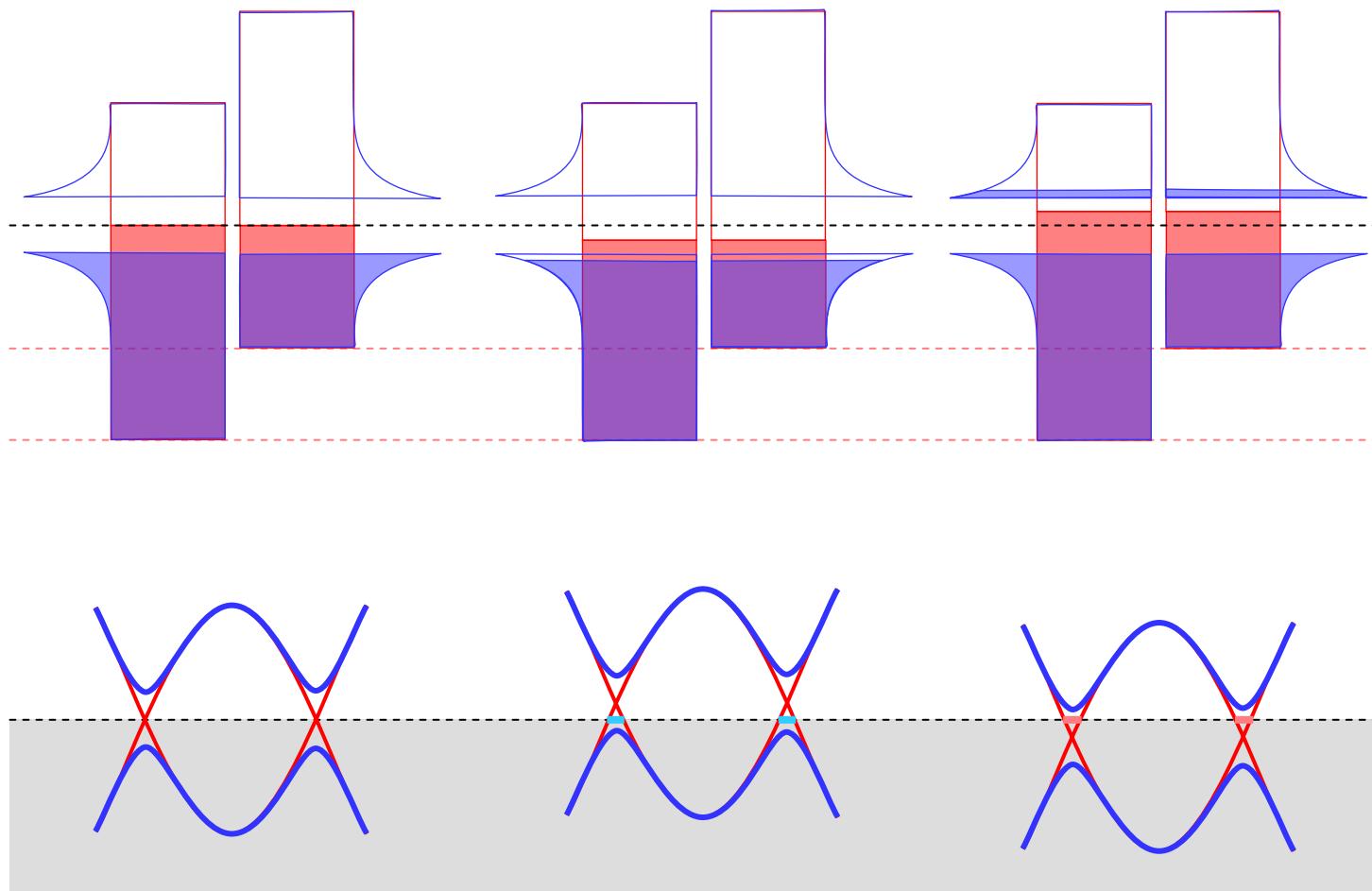
BFA: density of states



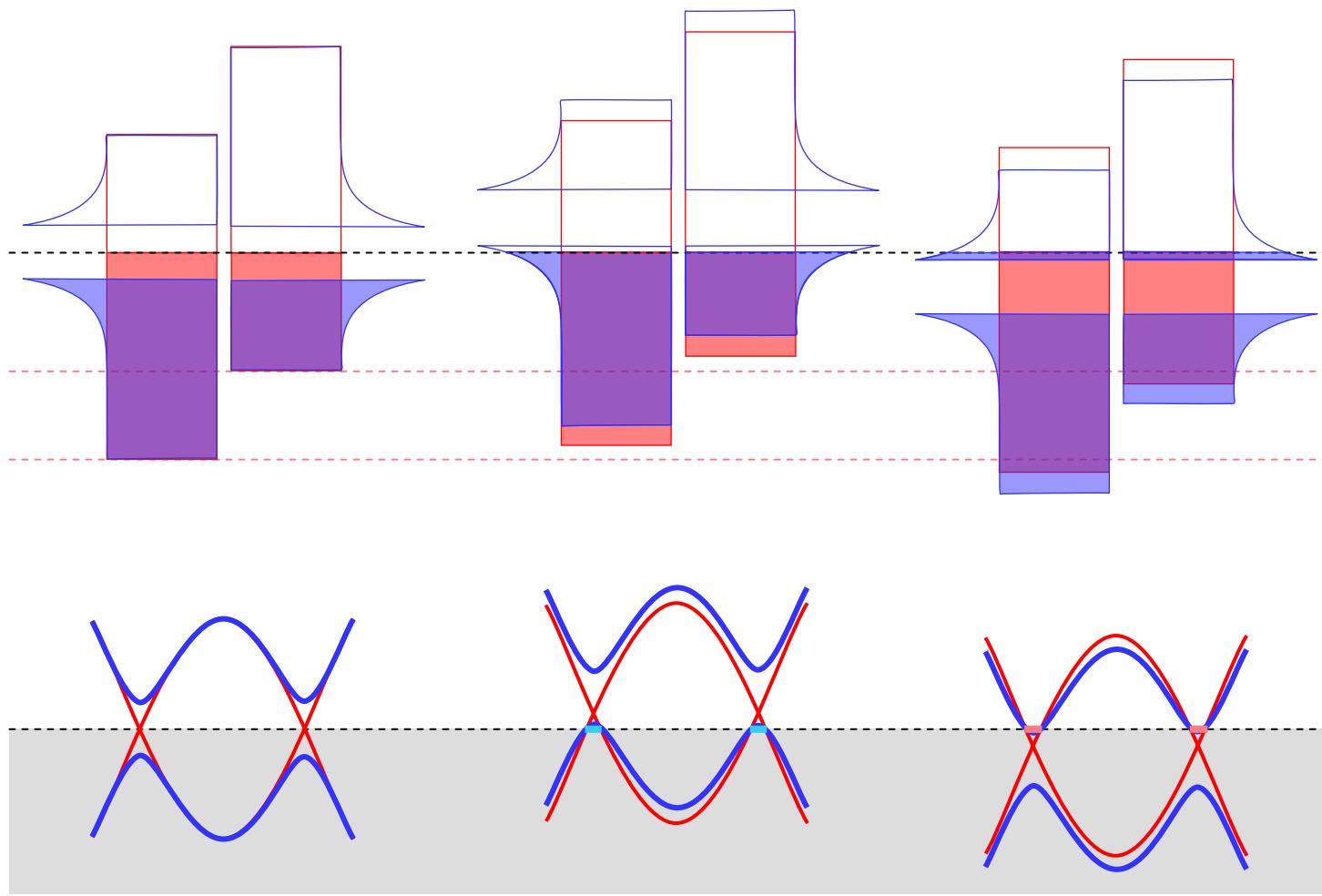
Generalized phase diagram



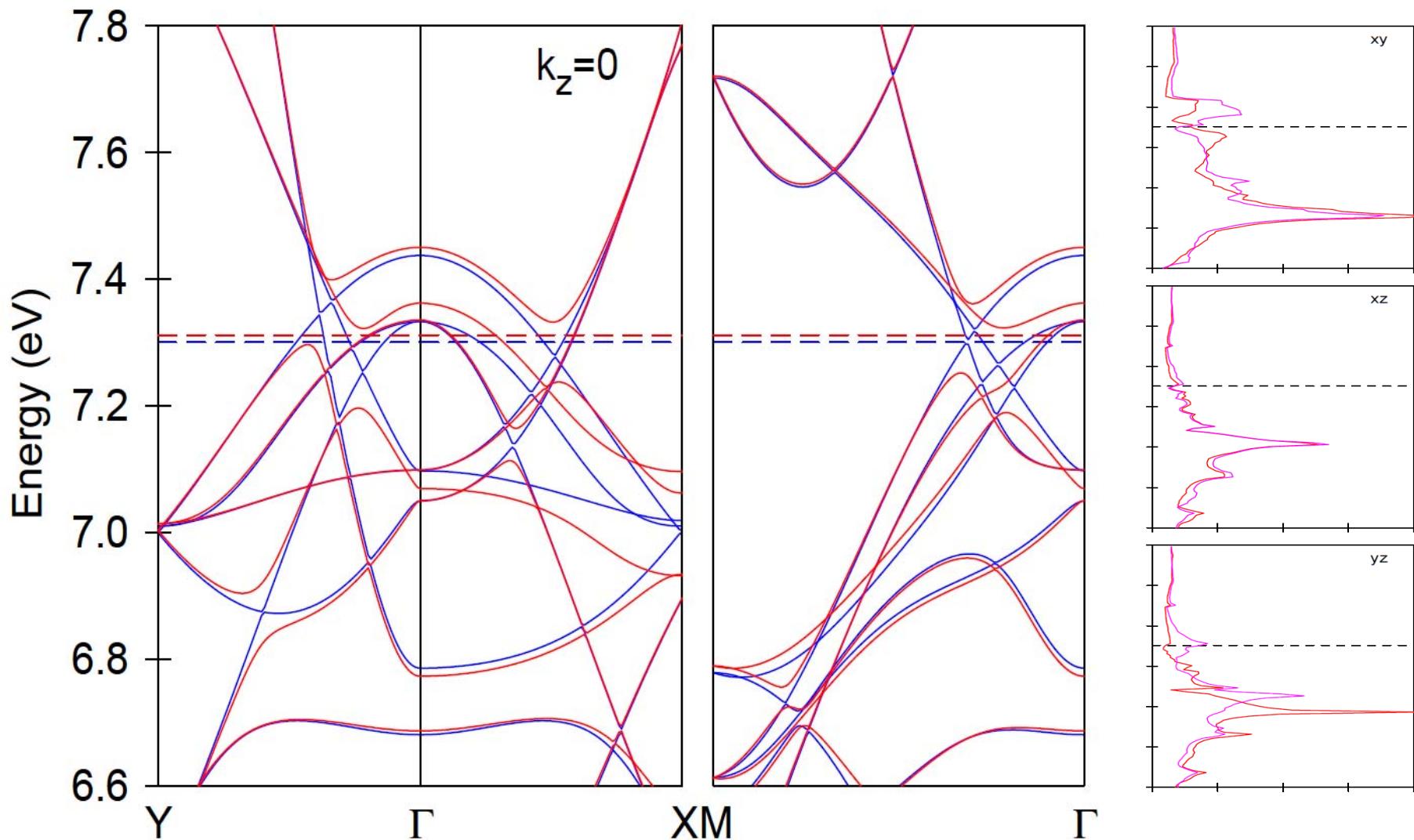
SC & SDW



SC & SDW



SC & SDW



Conclusions

- 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 T_c for different compounds seems to correlate with the position of the Van Hove singularities (Lifshitz transitions) for the xz - and yz -bands.
- Both the **renormalization** and **SDW** do increase the DOS at the Fermi level for dxz, yz - electrons.

THANK YOU