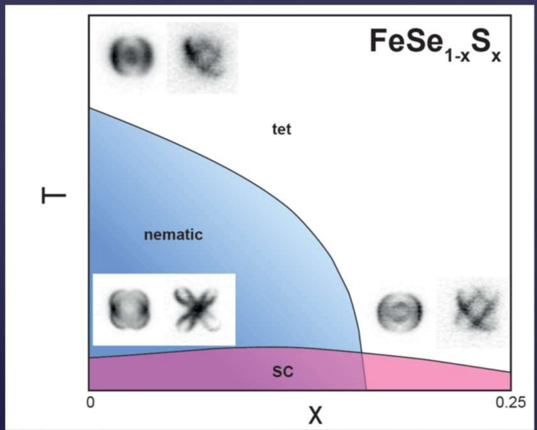
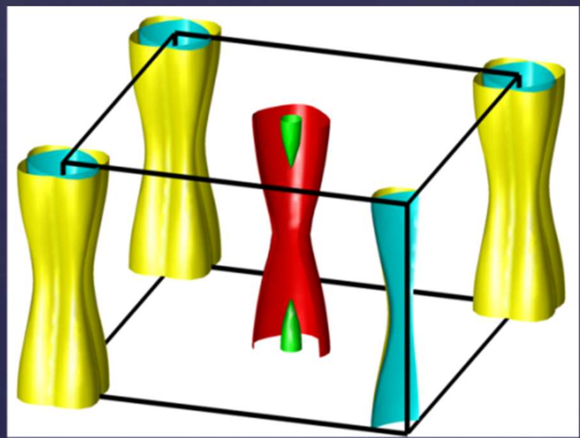
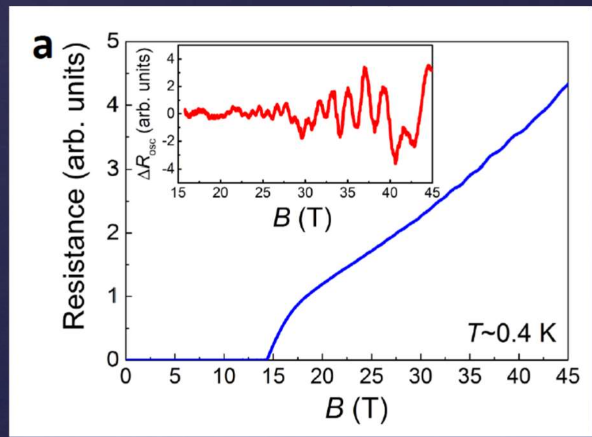
The key ingredients of the electronic structure of $FeSe_{1-x}S_x$. The role of chemical and applied pressure

Amalia Coldea

UNIVERSITY OF OXFORD

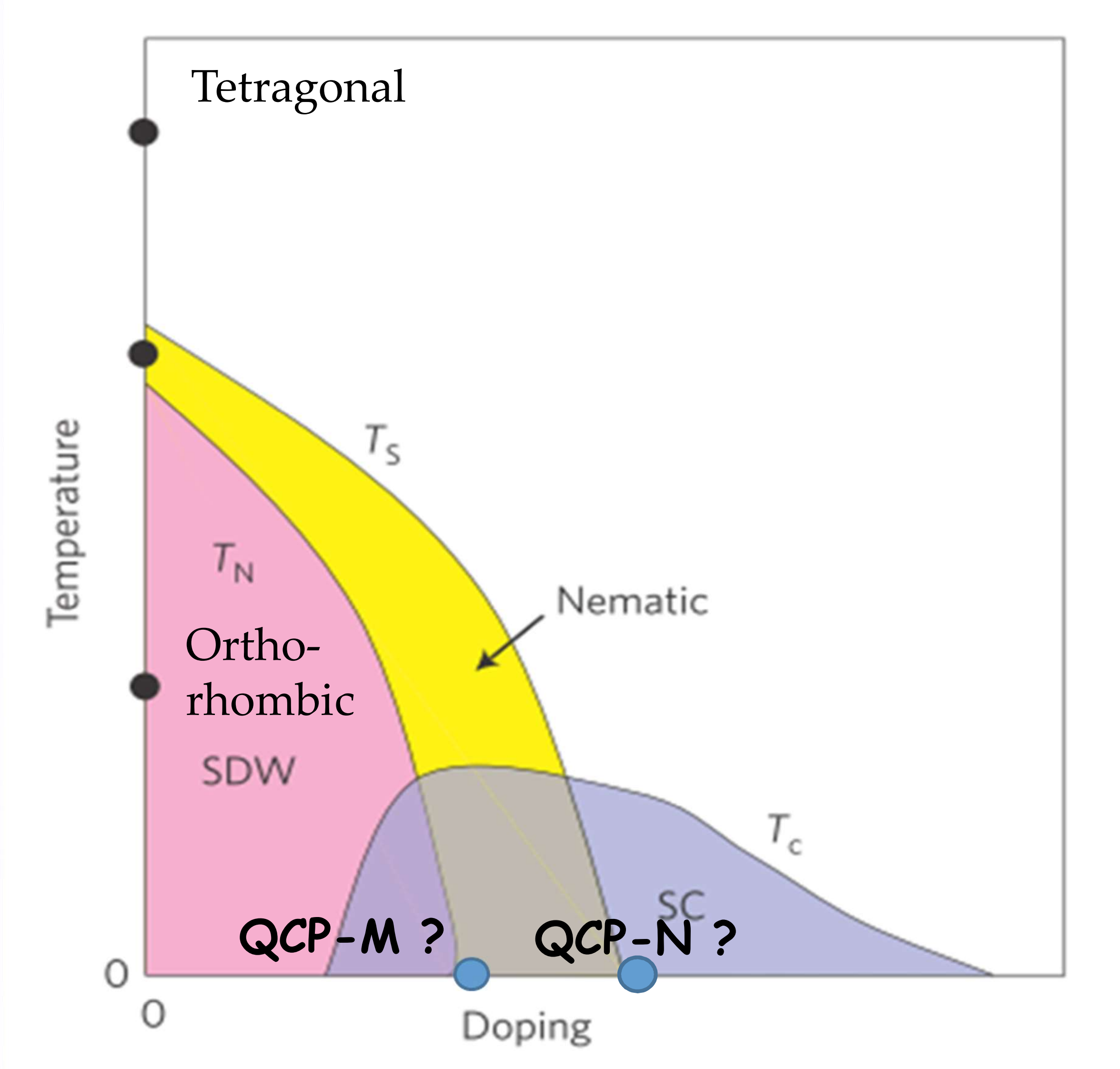


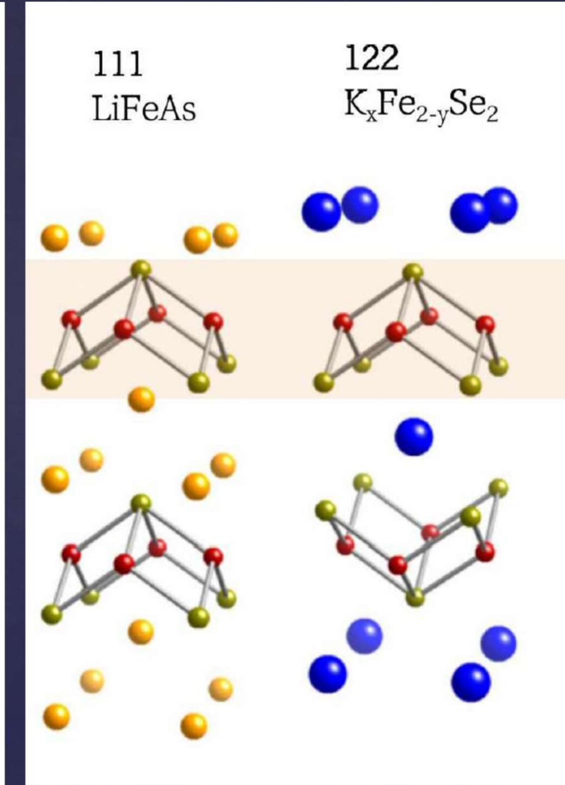




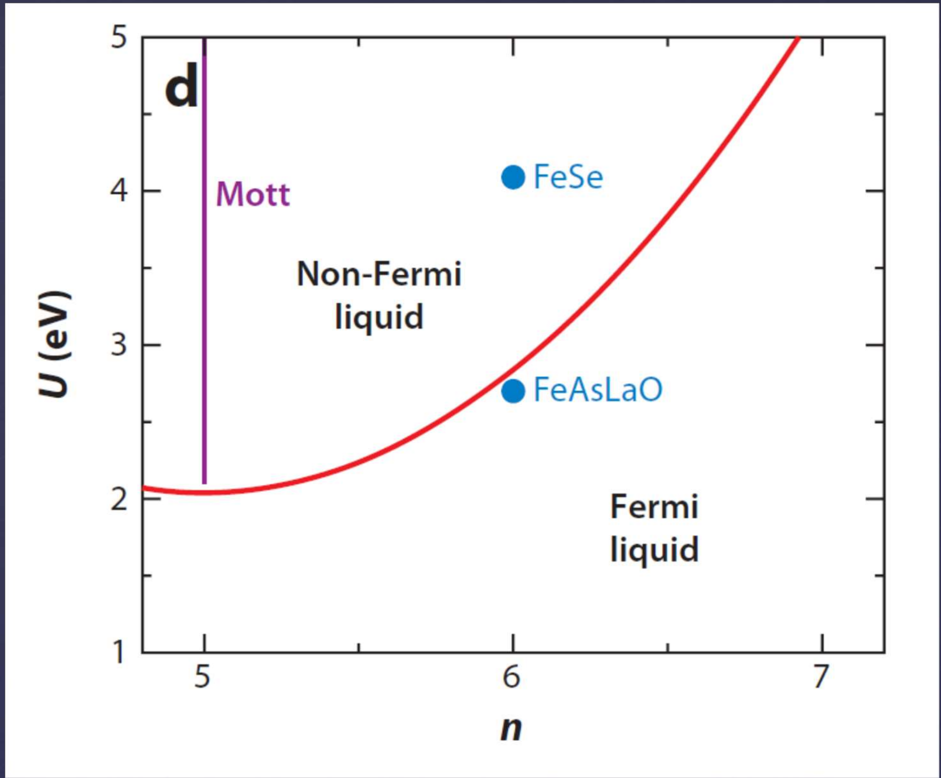
Intertwined Order and Fluctuations in Quantum Materials, KITP, 18 July 2017

Intertwined electronic orders in FeSC





Competing electronic phases in FeSC

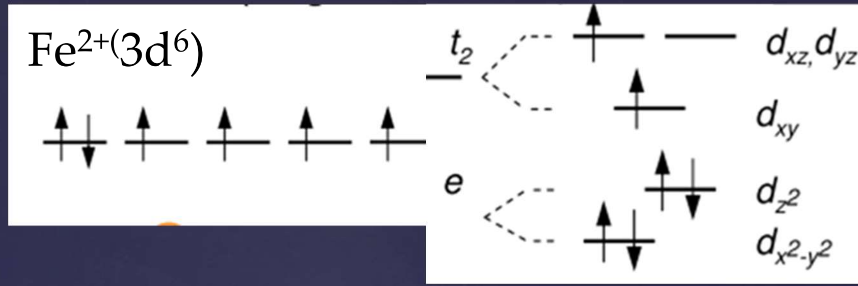


Hund's metals (J_{Hund}~0.35–0.4 eV)
(Electrons have dual nature, partly itinerant and partly localized)

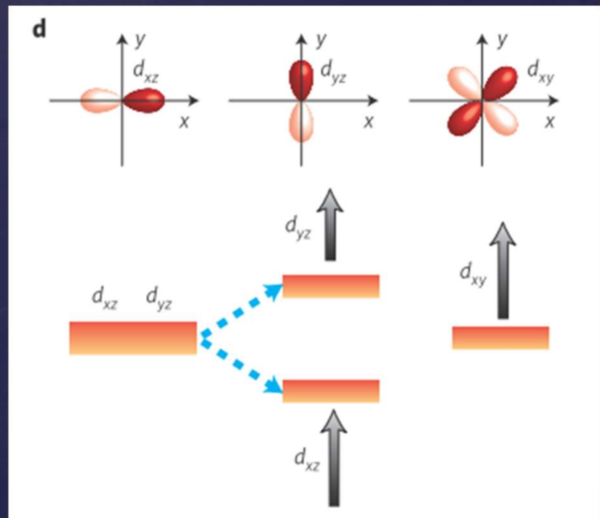
Orbitally-dependent renormalization effects
(dxy compared with dxz/yz)
Z. P. Yin, KH, G. Kotliar, Nature Materials (2011)

Annu. Rev. Condens. Matter Phys. 2013. 4:137–78

Hund's rule coupling

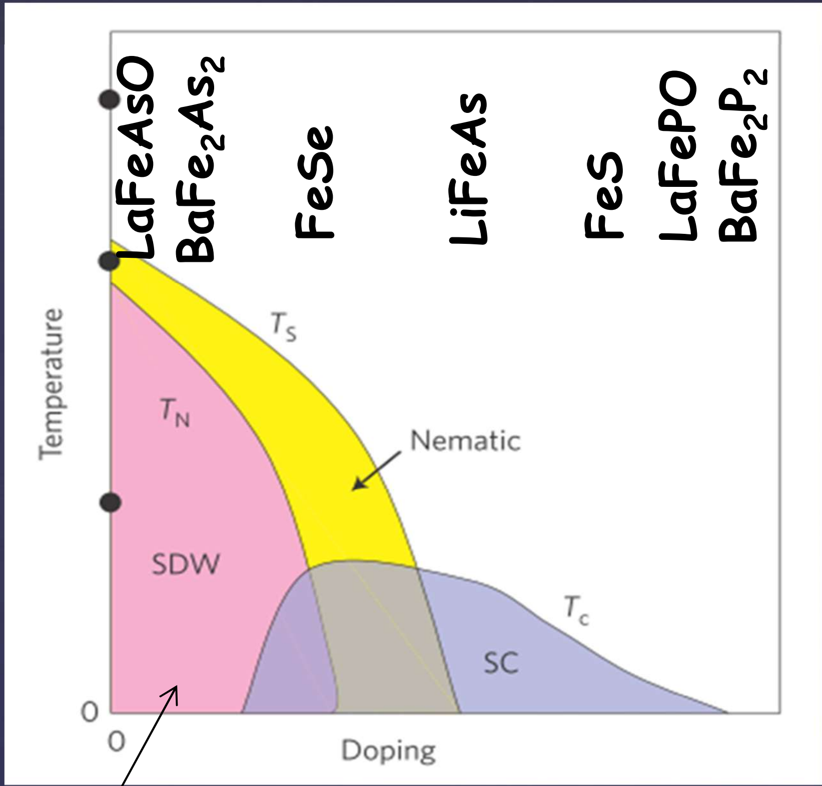


Orbital order in metallic systems



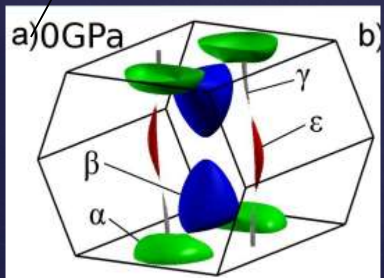
$$\Delta n = n_{xz} - n_{yz}$$

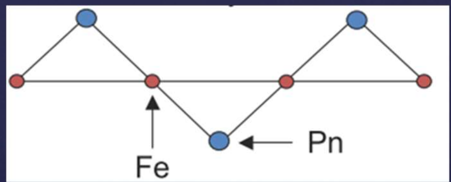
Generic phase diagram of isoelectronic FeSC



Hund's rule coupling, orbital content

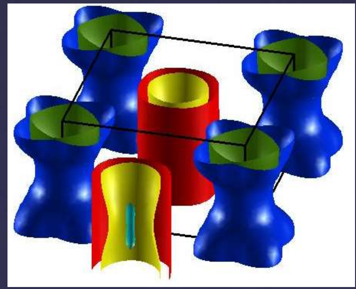
Bandwidth, W, chemical pressure (*c/a*)



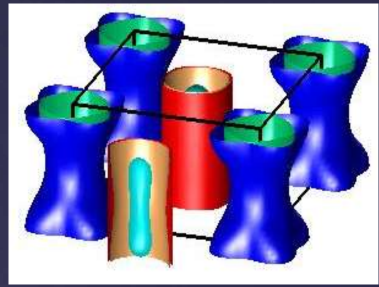


$$z_{As} > z_{P}$$

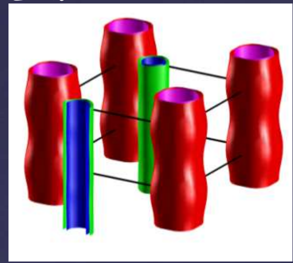
LiFeAs



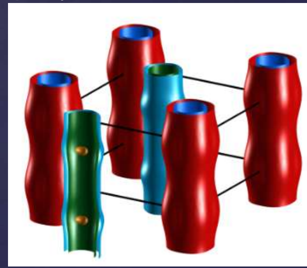
LiFeP



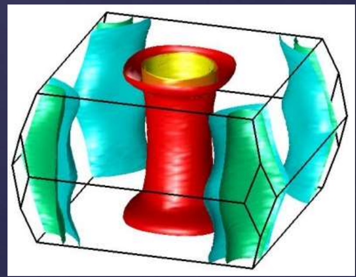
LaFeAsO



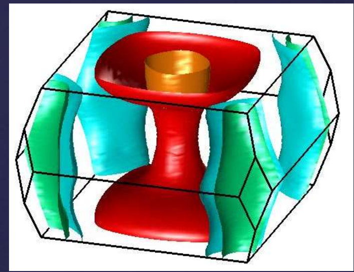
LaFePO



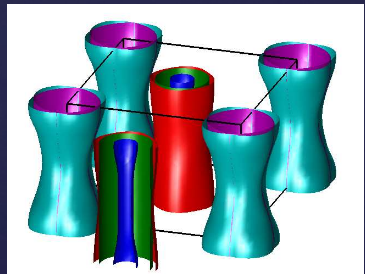
$BaFe_2As_2$



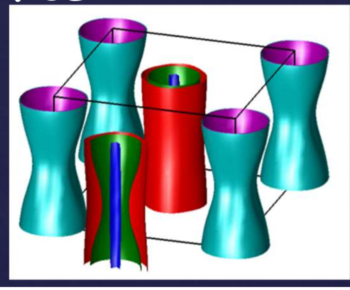
$BaFe_2P_2$



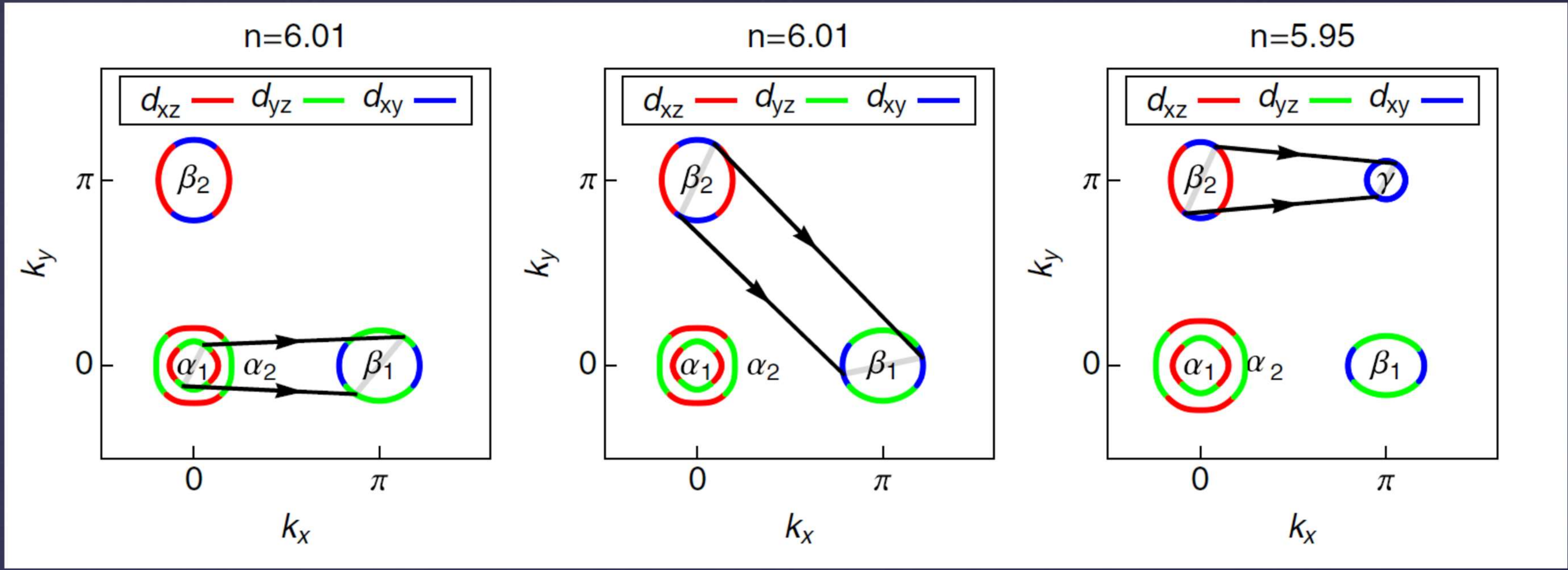
FeSe



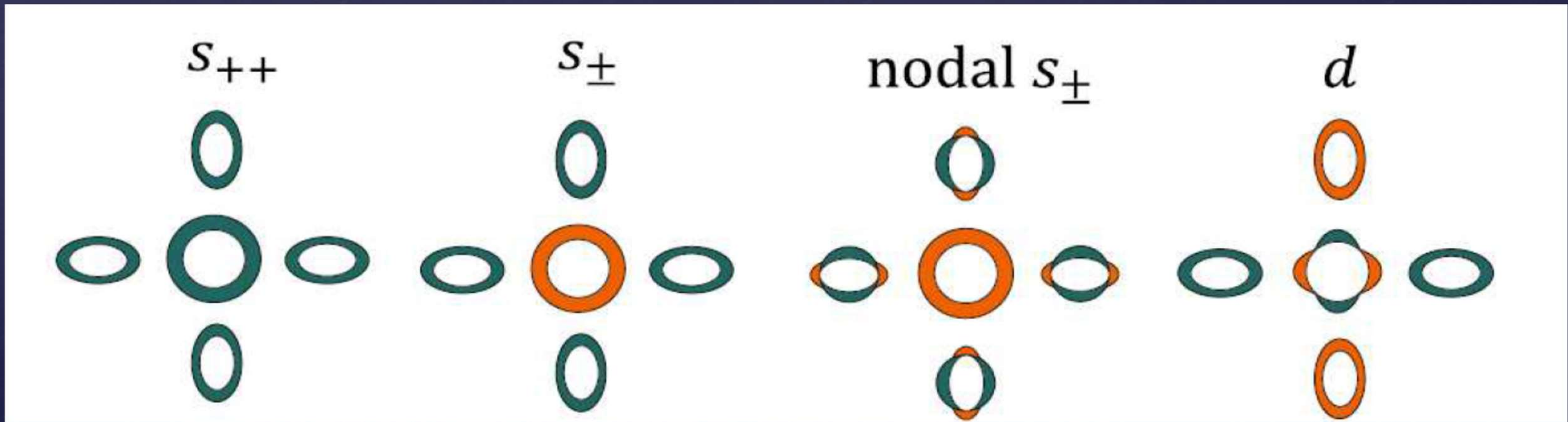
FeS



Nesting and the gap symmetry in FeSC

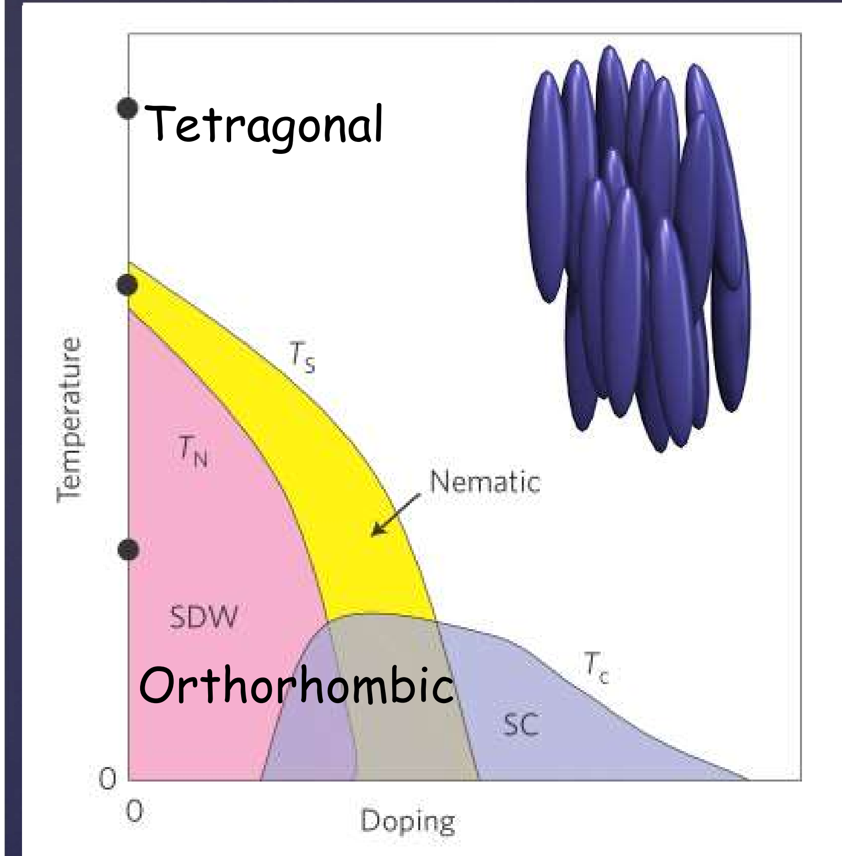


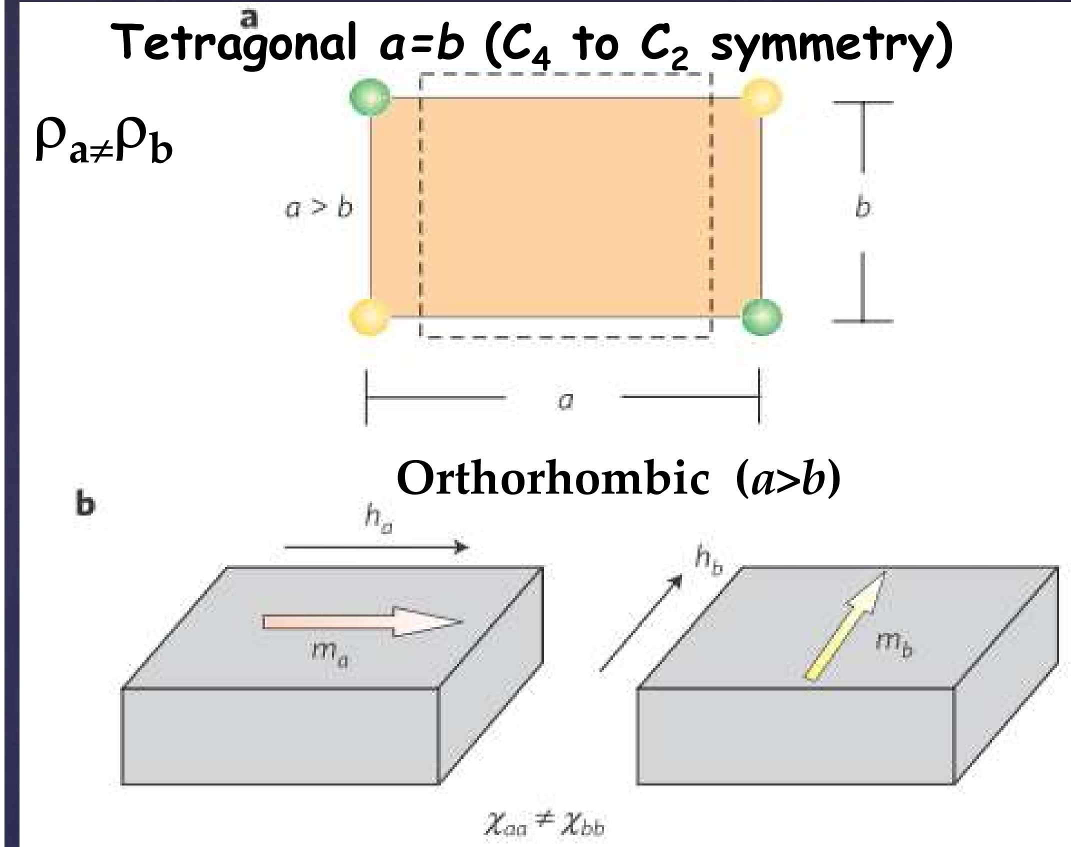
D. J. Scalapino Rev. Mod. Phys. **84**, 1383 (2012)



Hirschfeld, Korshunov, Mazin
Rep. Prog. Phys. **74** 124508 (2011)

The role of the nematic electronic state

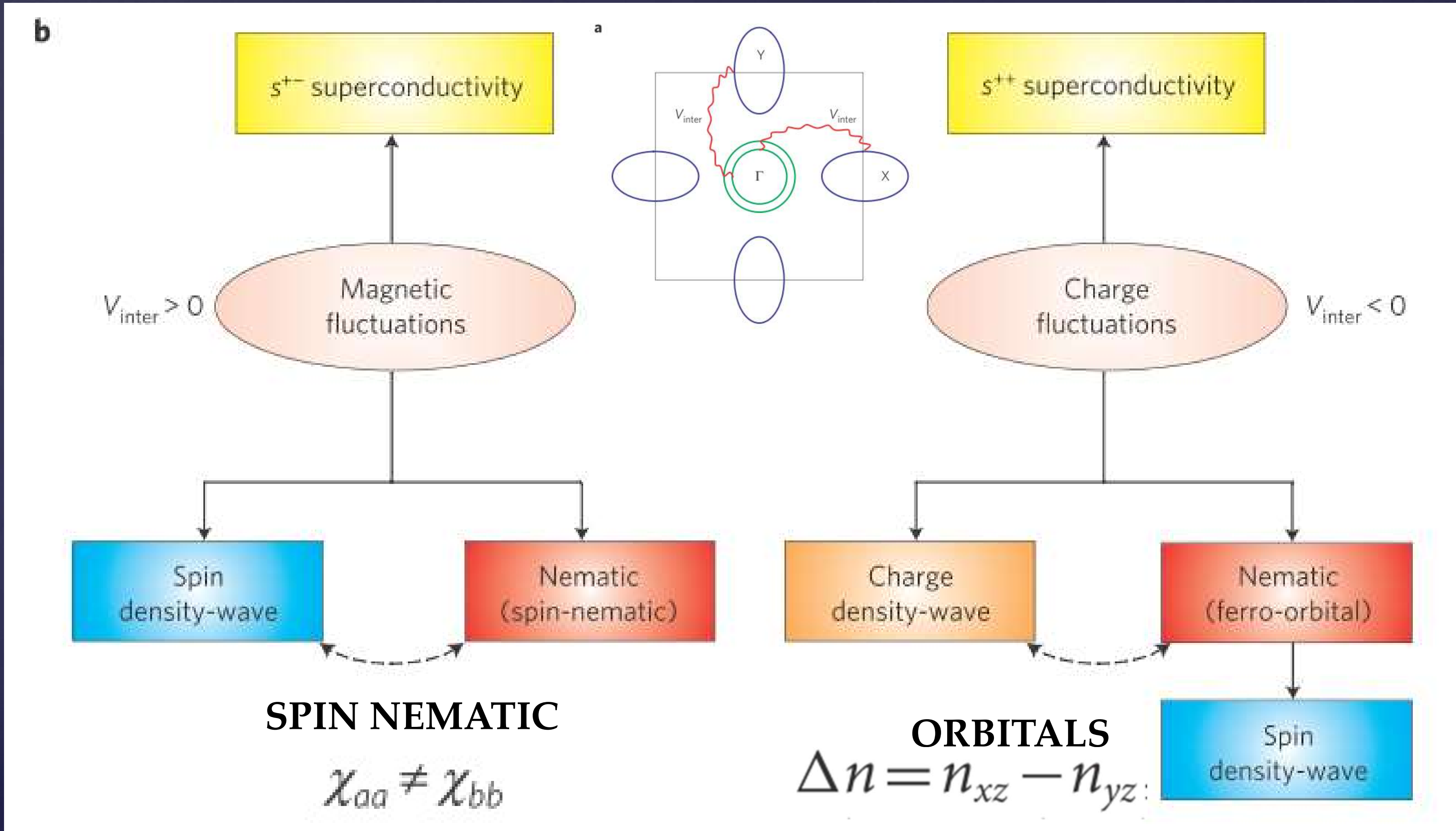




A nematic state is a form of electronic order that breaks the rotational symmetries without changing the translational symmetry of the lattice. Not a regular structural transition (tiny distortion) but it is the result of an electronically driven instability, orbital order or spin-driven Ising-nematic order.

NATURE PHYSICS | VOL 10 | FEBRUARY 2014

Superconductivity and nematicity

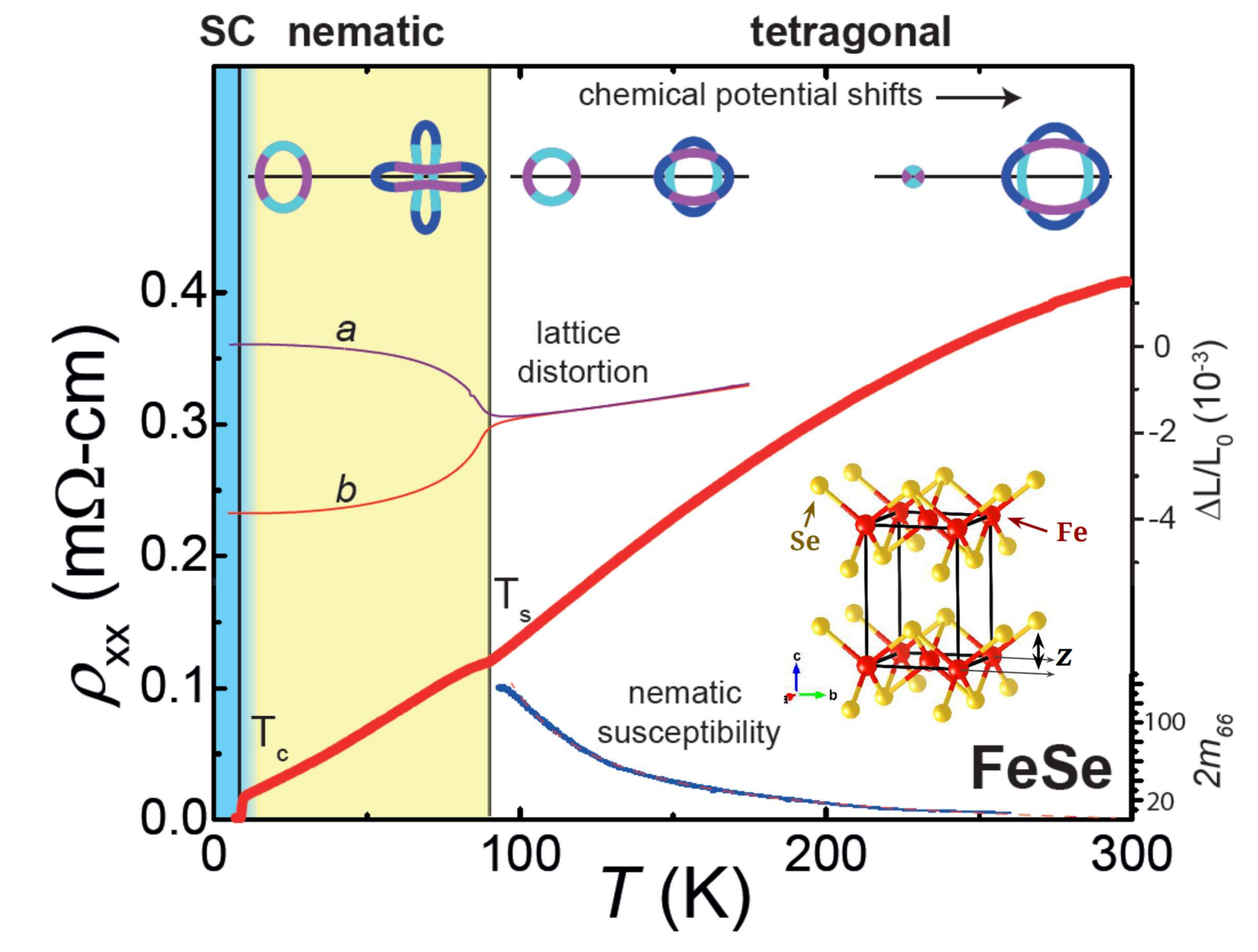


DOI: 10.1038/NPHYS2877

Nature Physics, 10, 97 (2014)

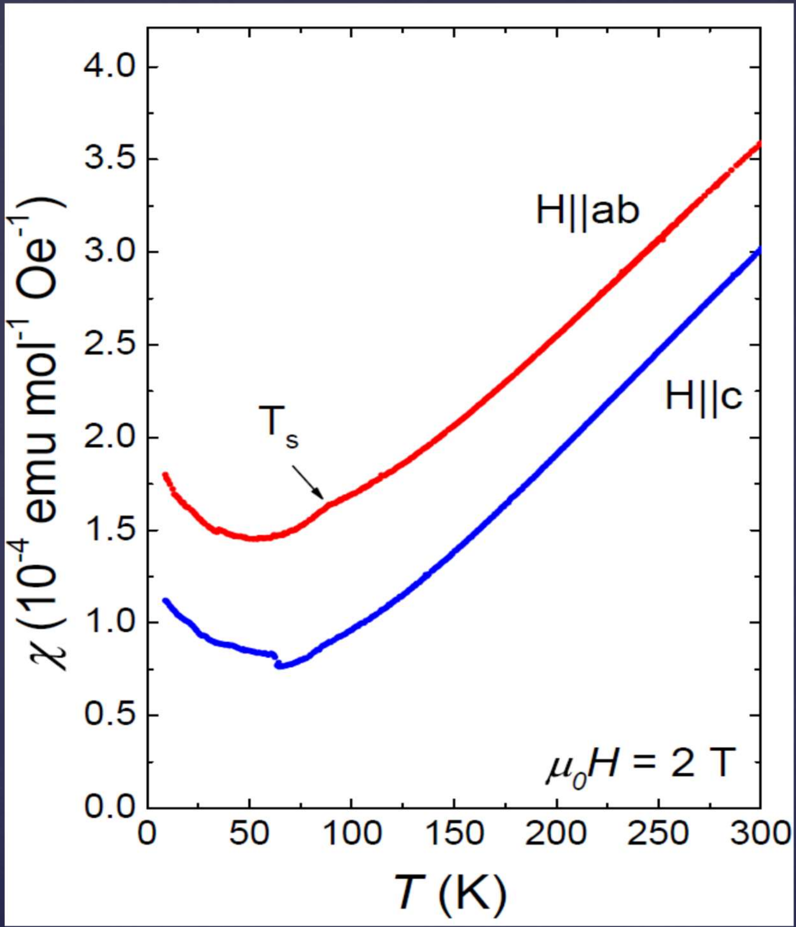
I. Introduction to FeSe

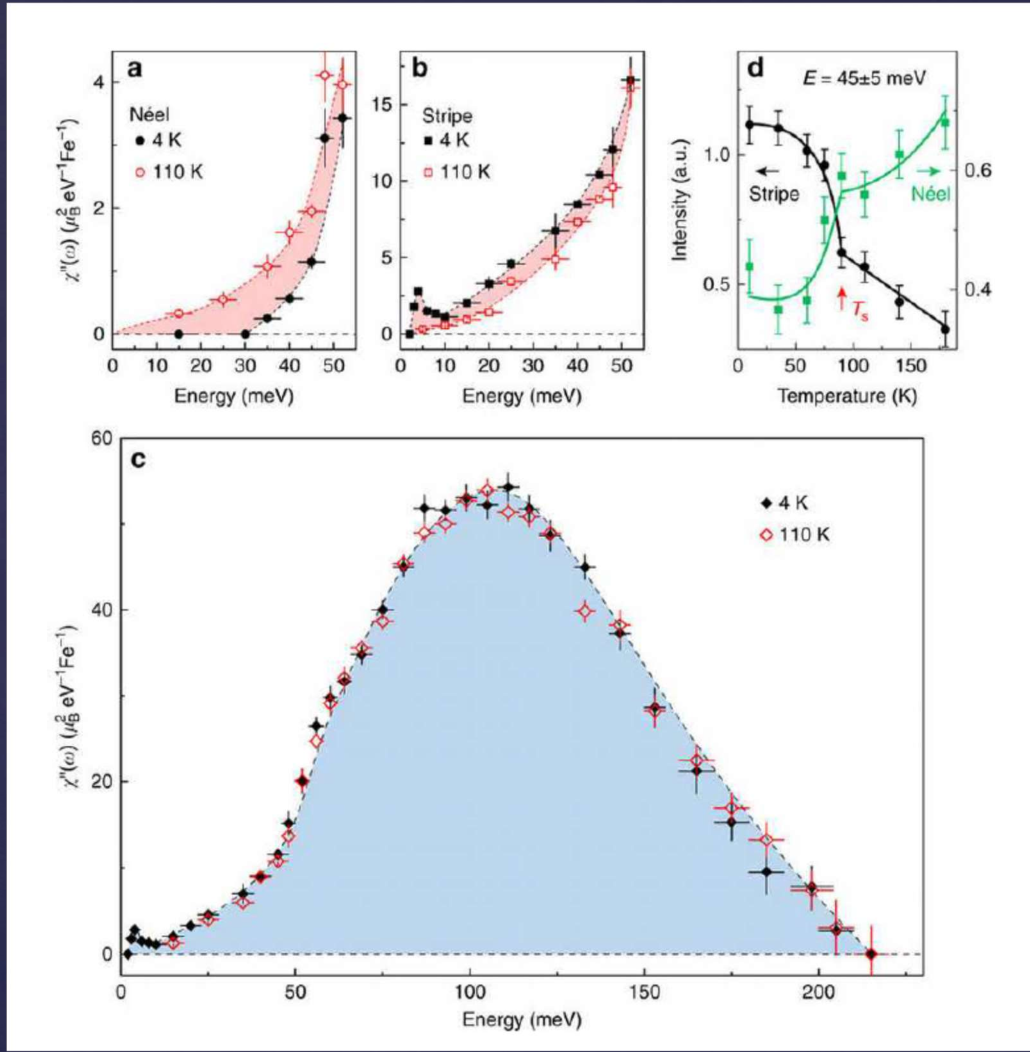
FeSe- a nematic superconductor ?



Coldea &Watson, arXiv.1706.00338, Annual Reviews Condensed Matter 2018

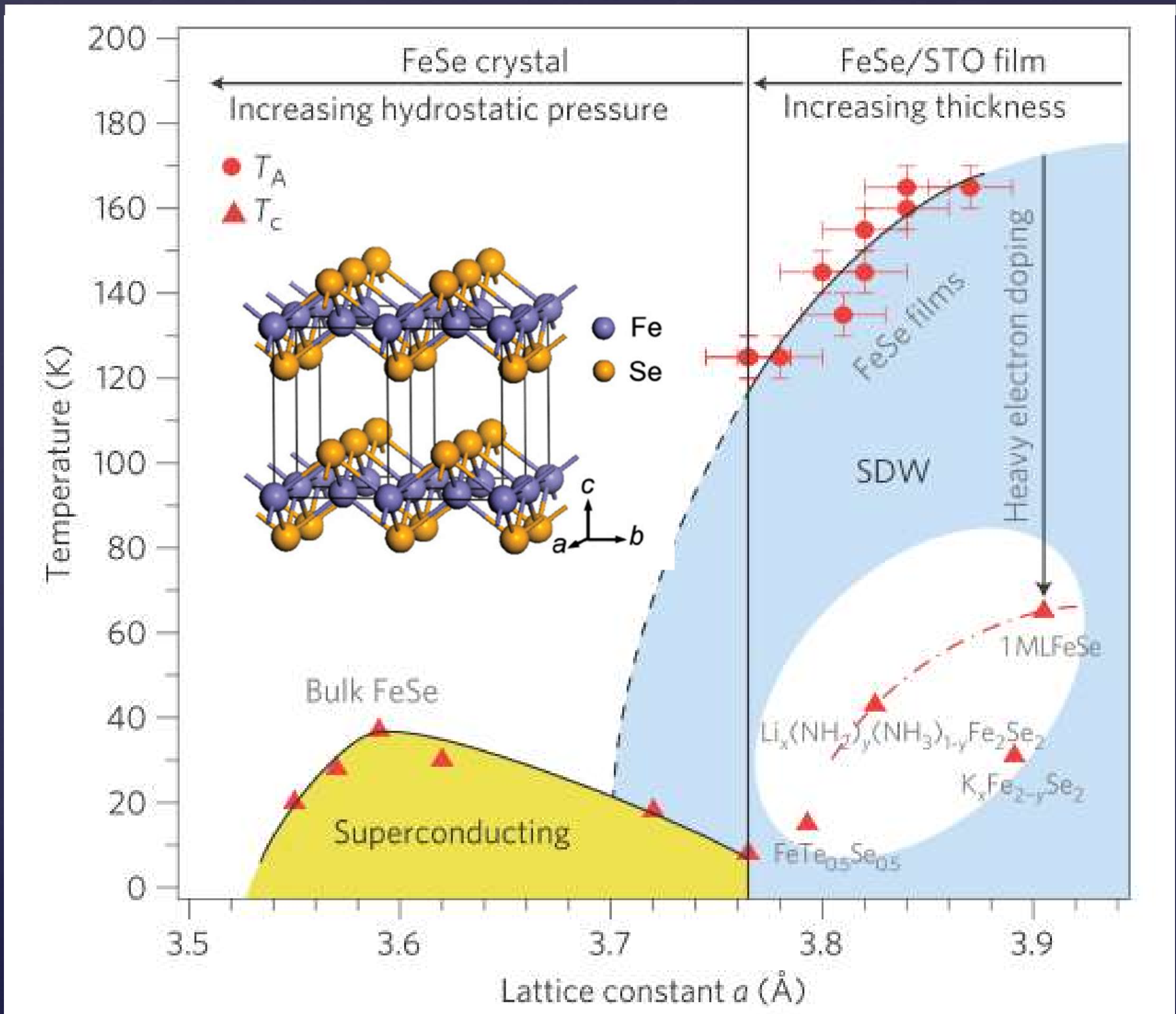
FeSe- no long range magnetism. "Frustrated" spin fluctuations ?





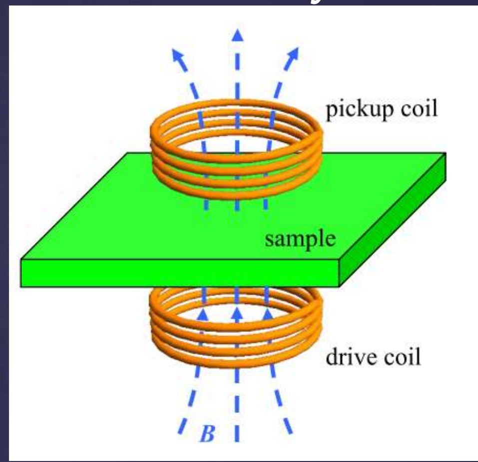
Wang et al., Nat. Commun. **7**, 12182 (2016)

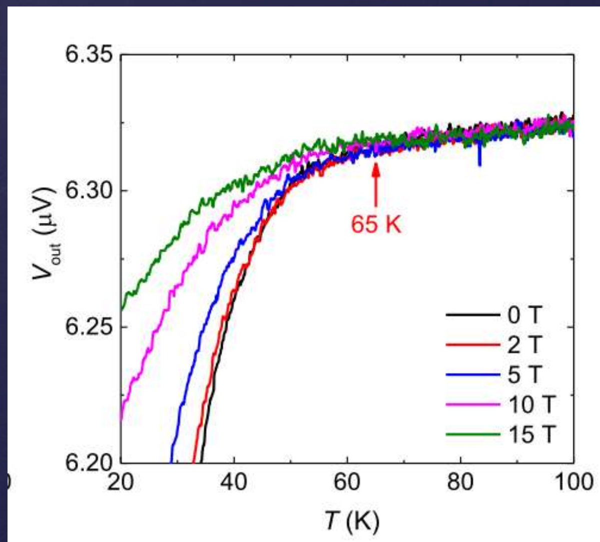
Tc superconductivity up to 75K in monolayer of FeSe grown on SrTiO3



NATURE MATERIALS | VOL 12 | JULY 2013 |

FeSe monolayer/STO

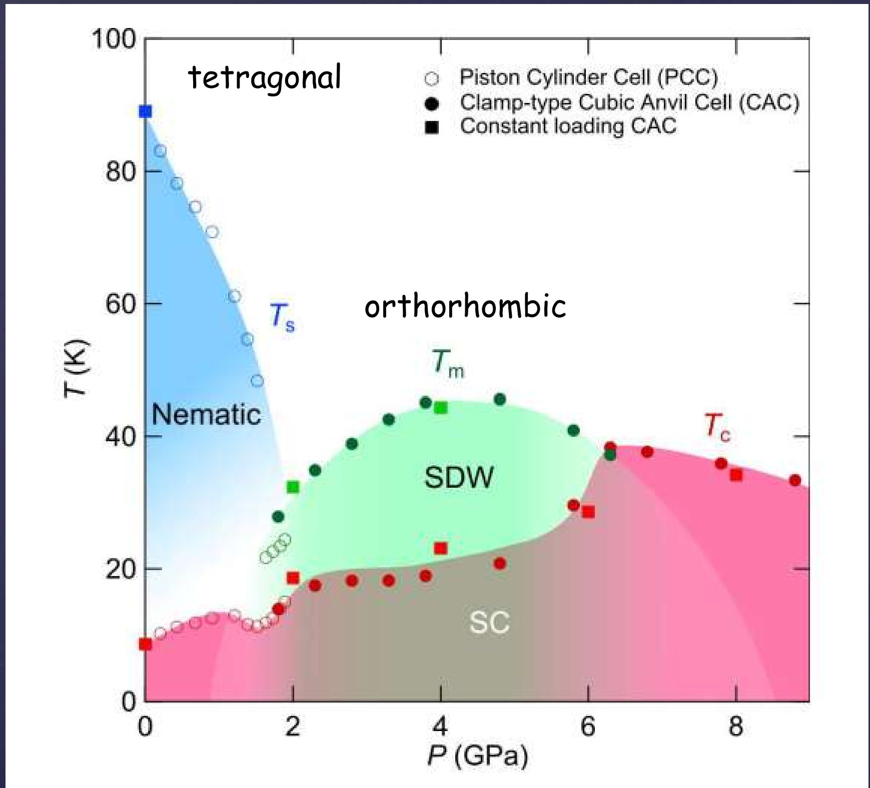




Science Bulletin 60 (14), 1301-1304 (2015)

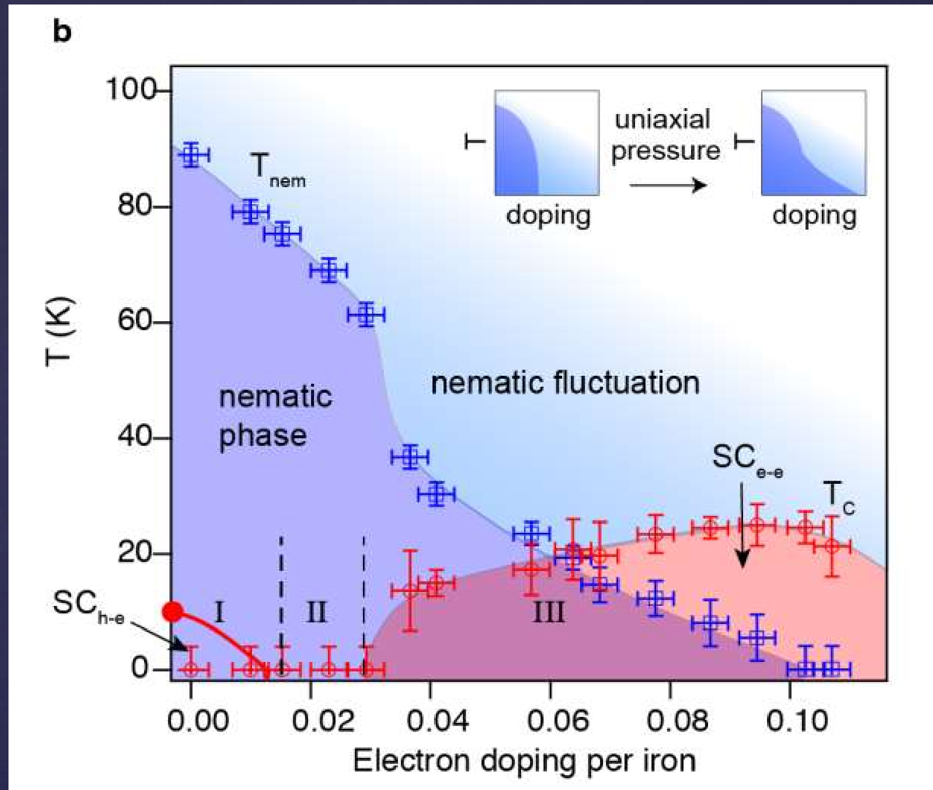
Enhancing superconductivity in bulk FeSe

applied external pressure



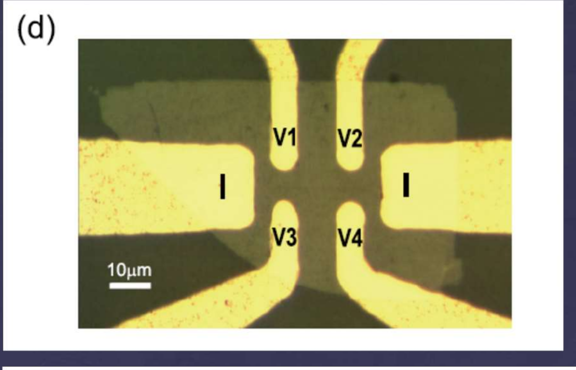
J.P. Sun *et al.*, Nat. Commun. 7, 12146 (2016)

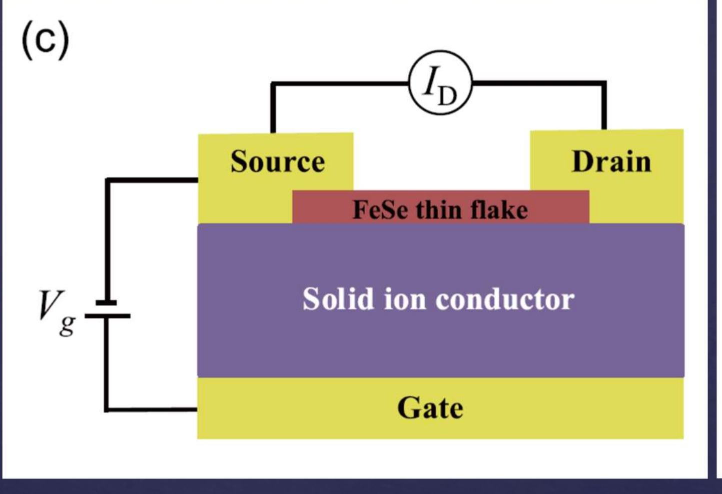
in-situ electron doping with K ions

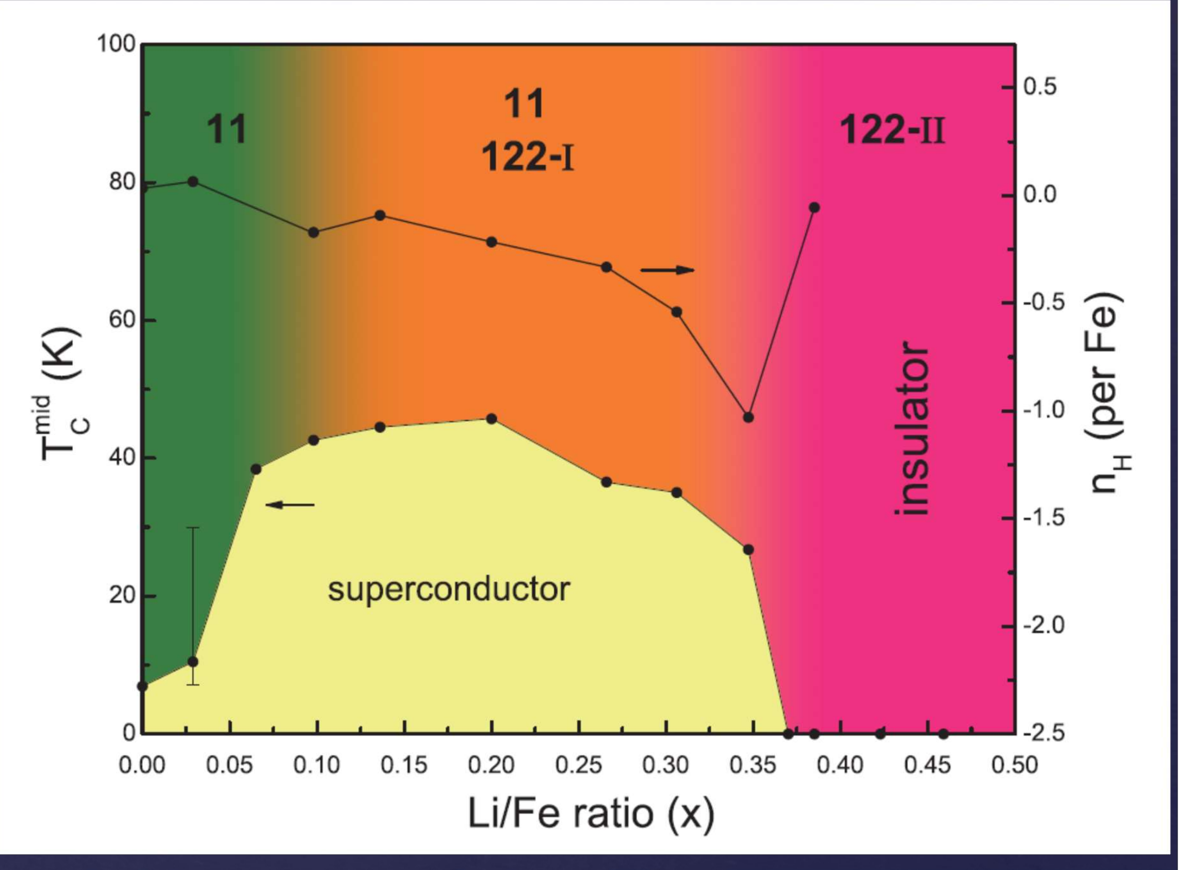


Z. R. Ye et al., arXiv:1512.02526 (2015)

Enhancing superconductivity in thin flakes of FeSe





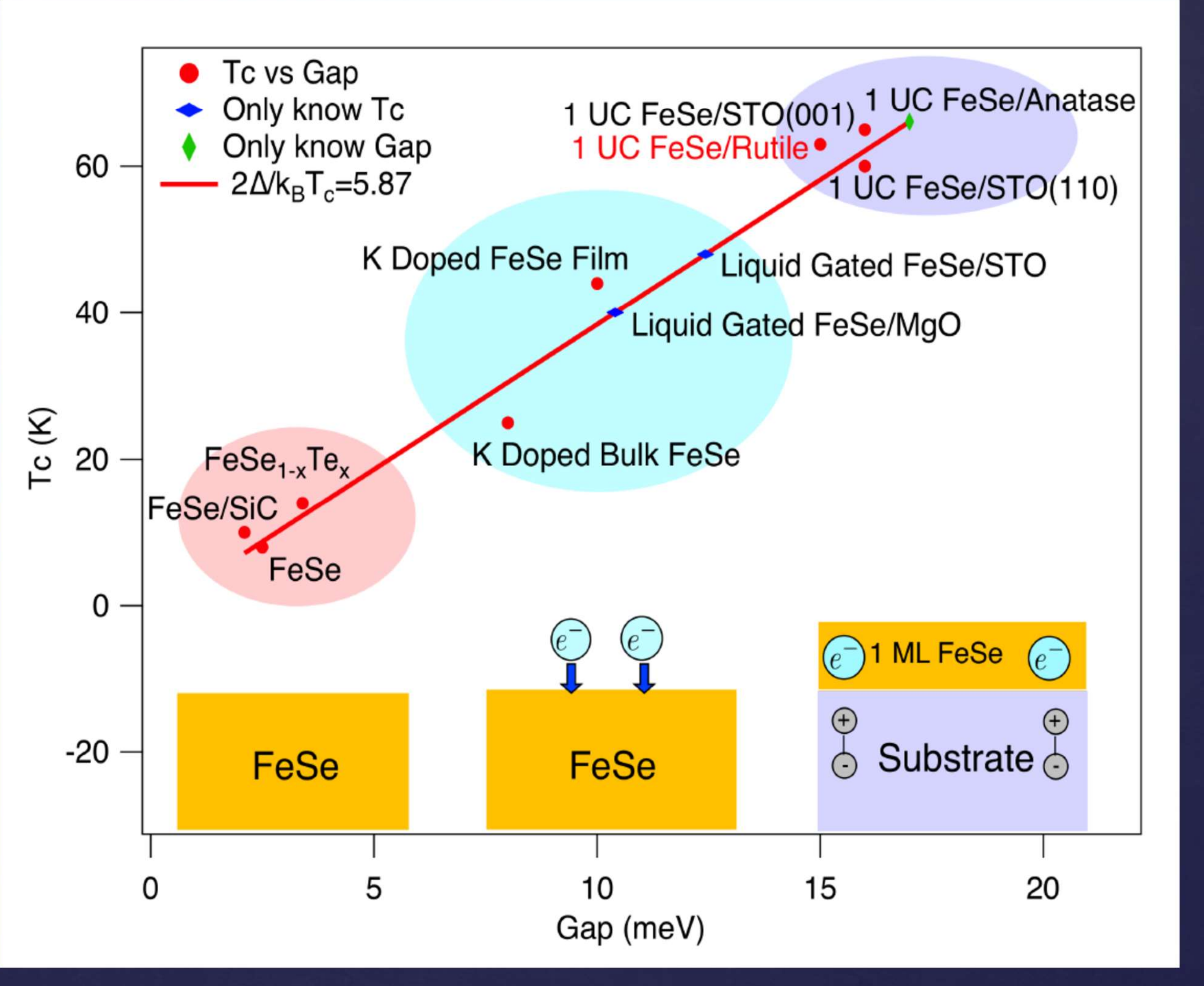


PHYSICAL REVIEW B **95**, 020503(R) (2017)

Superconductivity of FeSe

bulk

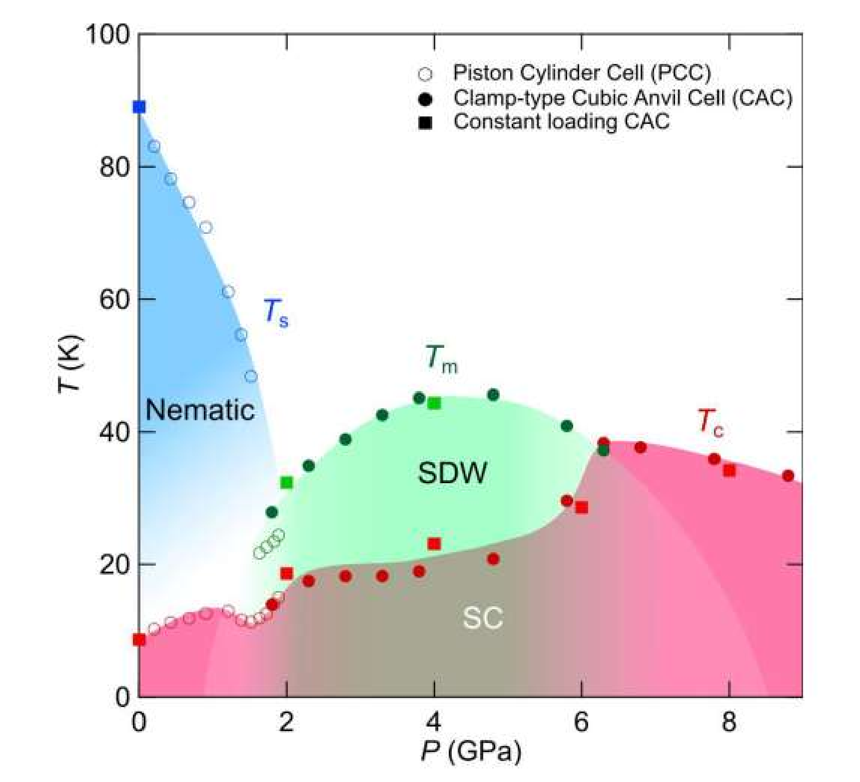
interfacial



Slavko Rebec et al., PRL. 118, 067002 (2017)

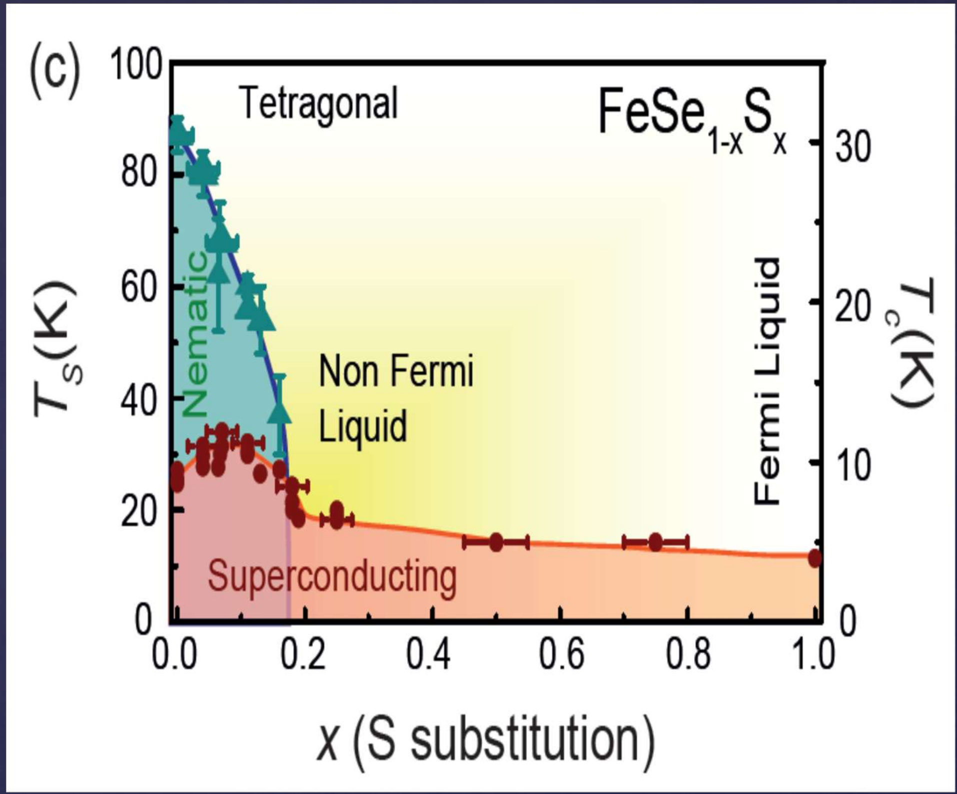
Chemical versus applied pressure in bulk FeSe

applied external pressure



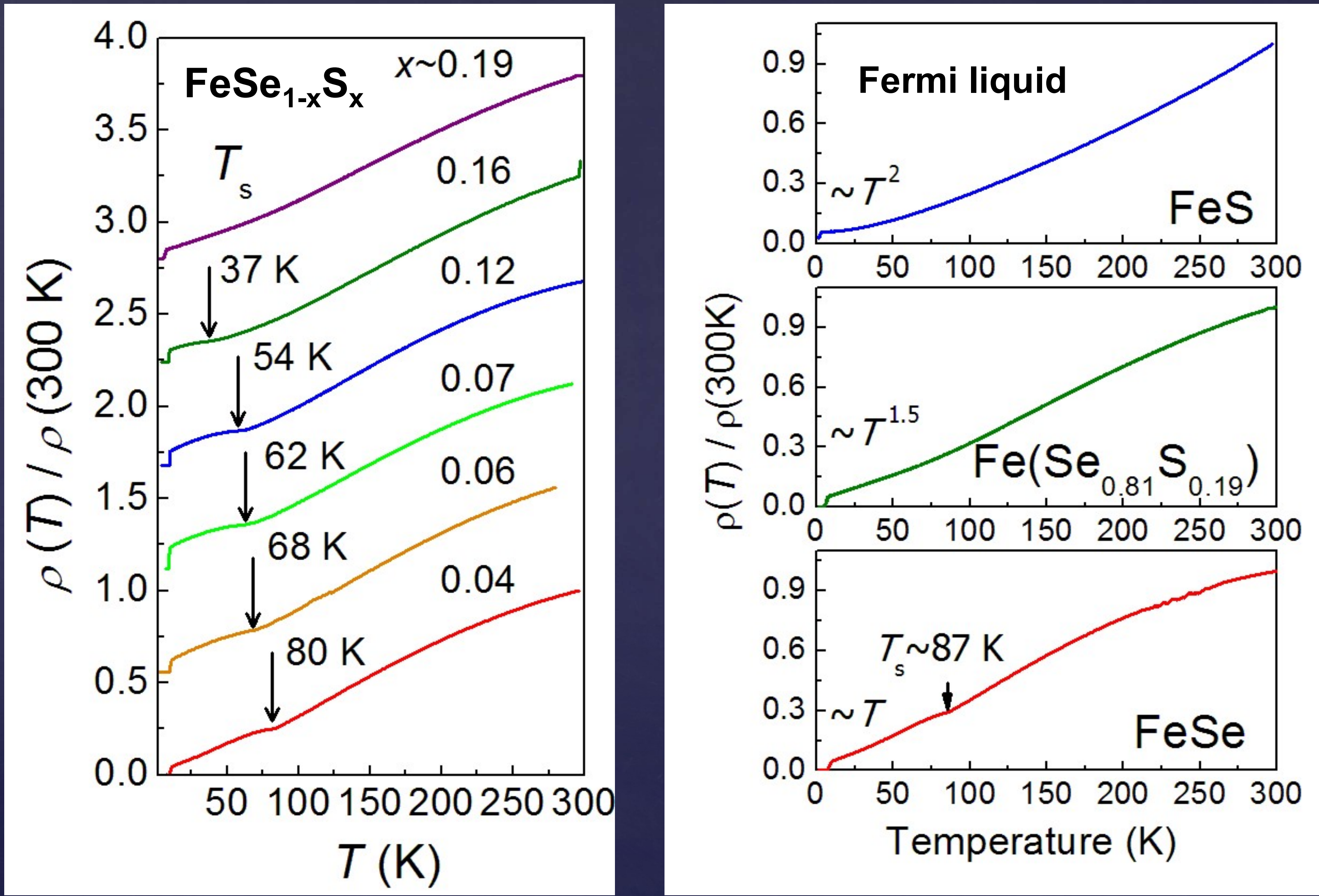
J.P. Sun *et al.*, Nat. Commun. 7, 12146 (2016)

chemical pressure

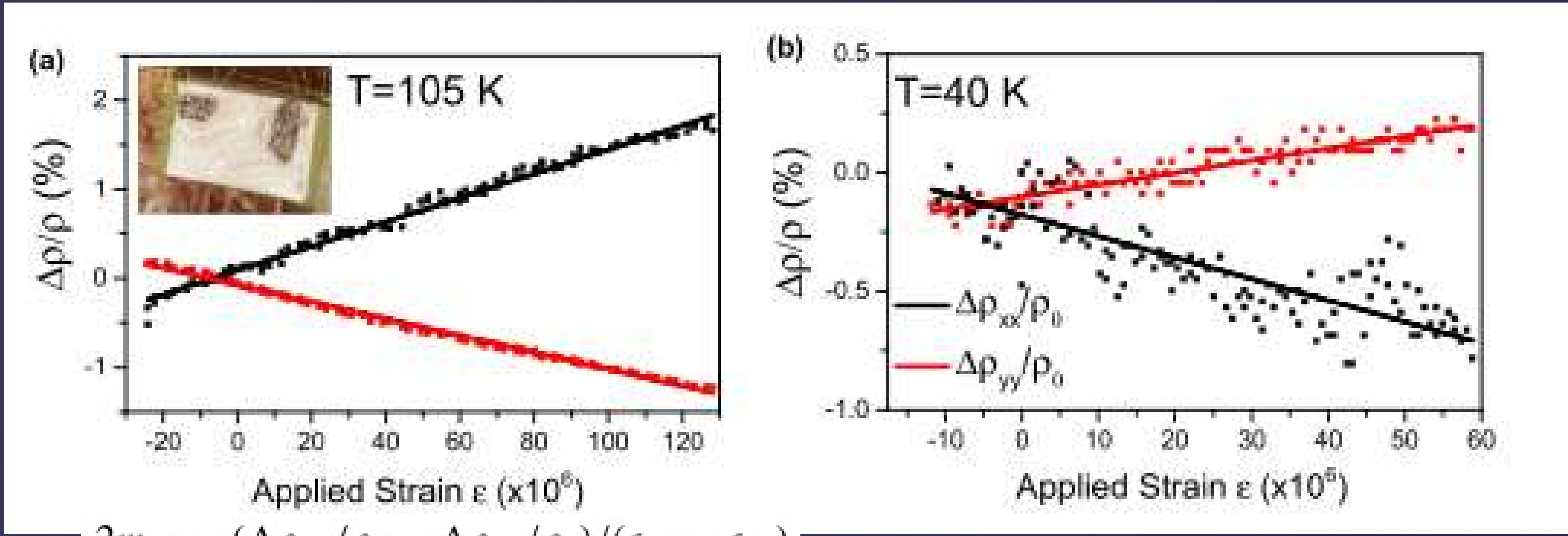


P. Reiss et al. AIC , arXiv:1705.11139

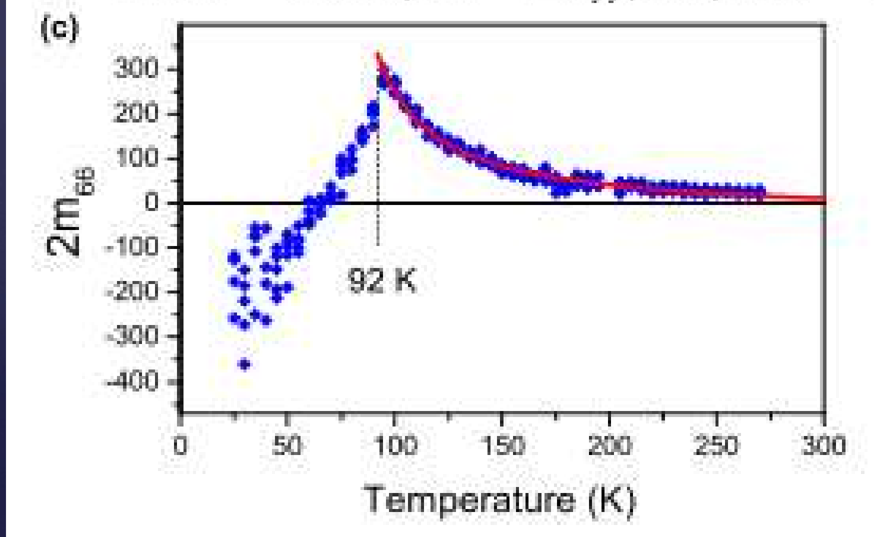
Strange metal behavior of $Fe(Se_{1-x}S_x)$

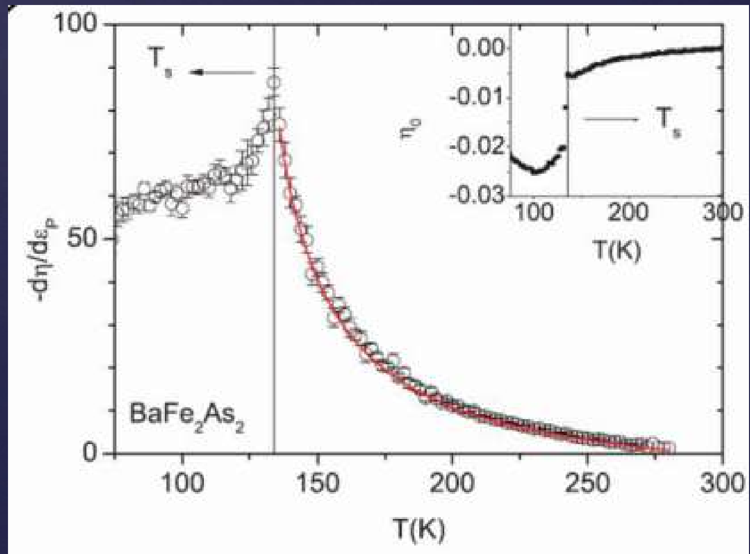


Nematic susceptibility of FeSe



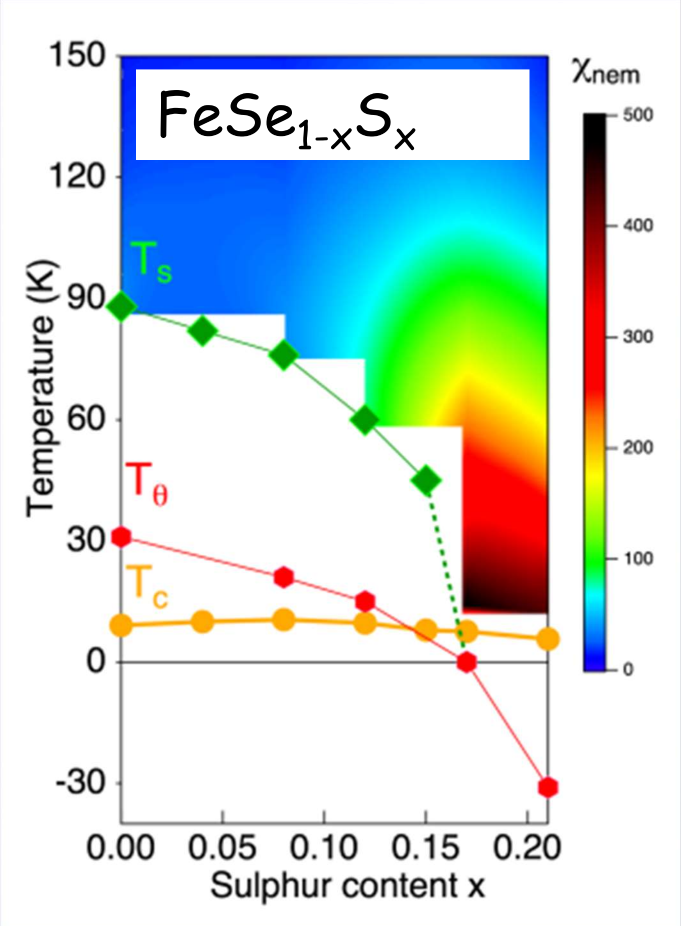
$$2m_{66} = (\Delta\rho_{xx}/\rho_0 - \Delta\rho_{yy}/\rho_0)/(\epsilon_{xx} - \epsilon_{yy}),$$

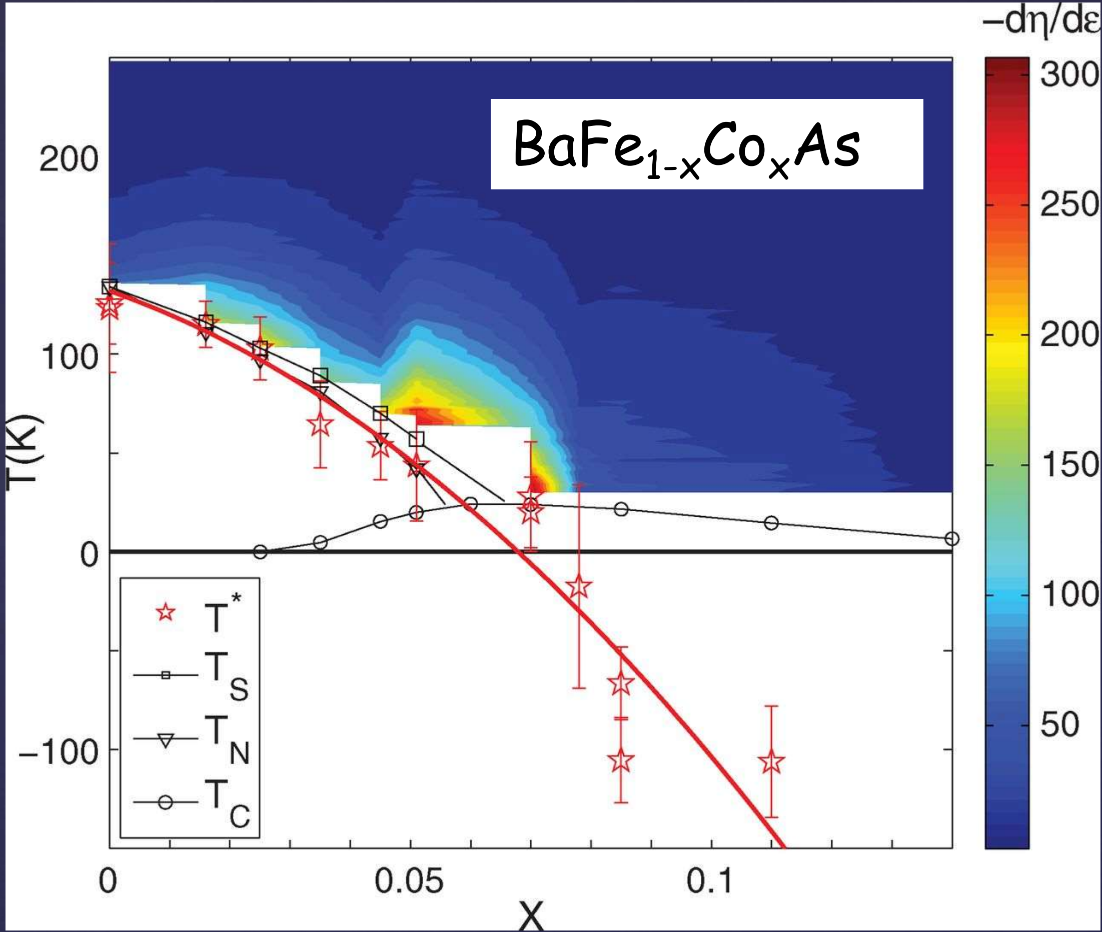




N. Davies, M. D. Watson, AIC,PRB 91, 155106 (2015)

Nematic criticality in $Fe(Se_{1-x}S_x)$





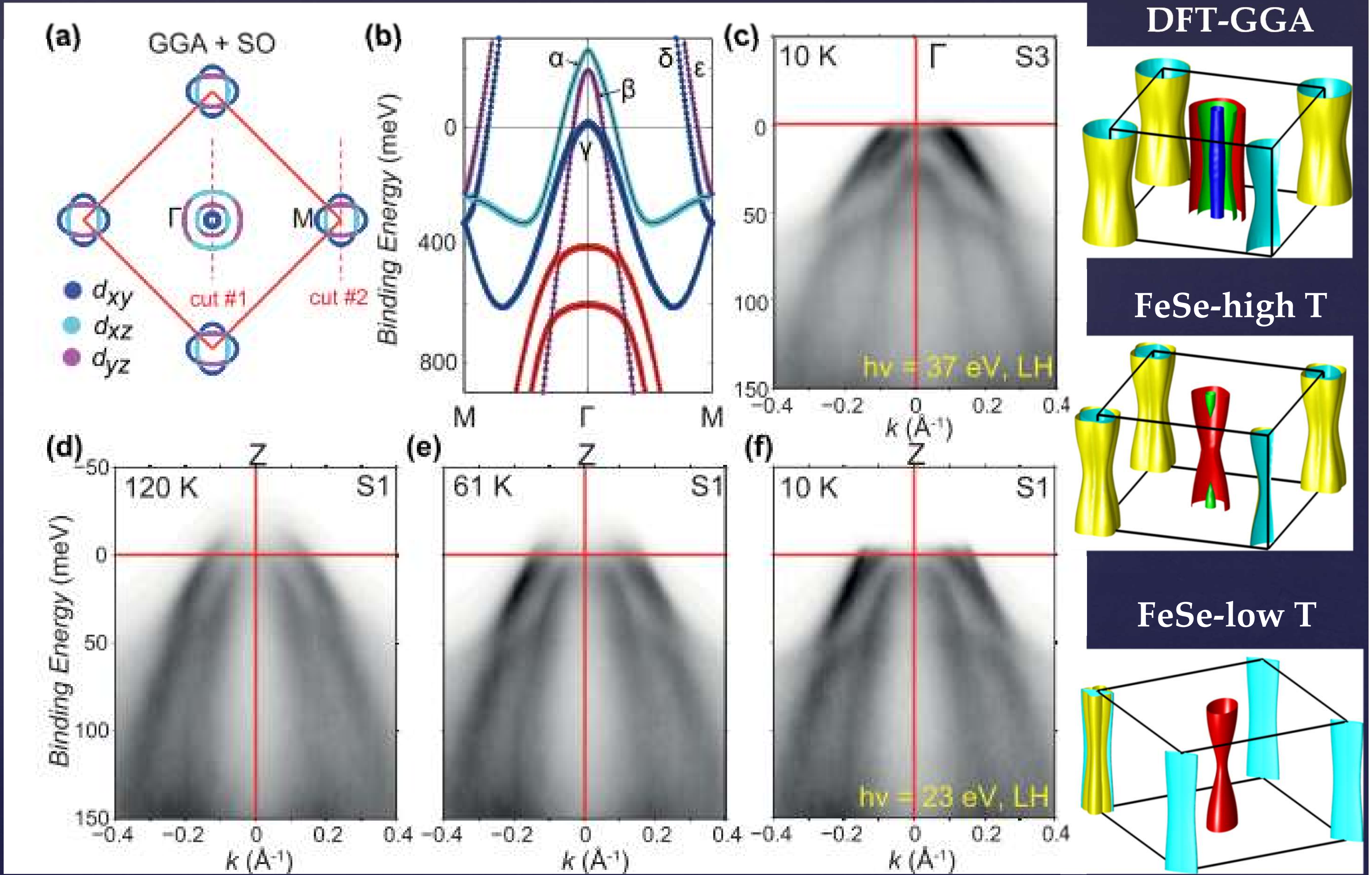
S. Hosoi *et al.*, PNAS 113, 8139 (2016)

J. Chu, Science, 337, 710 (2012)

II. ARPES studies in $Fe(Se_{1-x}S_x)$

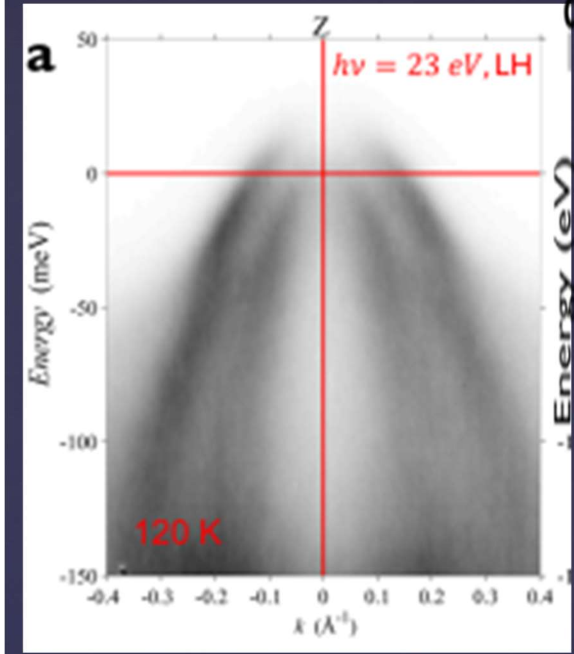
M. D. Watson et al., AIC,PRB 91, 155106 (2015); PRB 92, 121108 (2015);
PRB 94, 201107 (2016); PRB 95, 081106 (2017);
P. Reiss et al. AIC , arXiv:1705.11139 (2017)

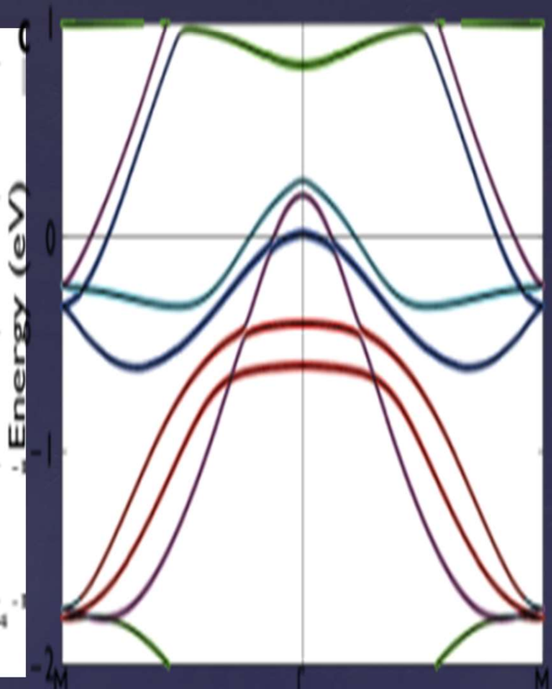
ARPES studies on FeSe: Hole bands

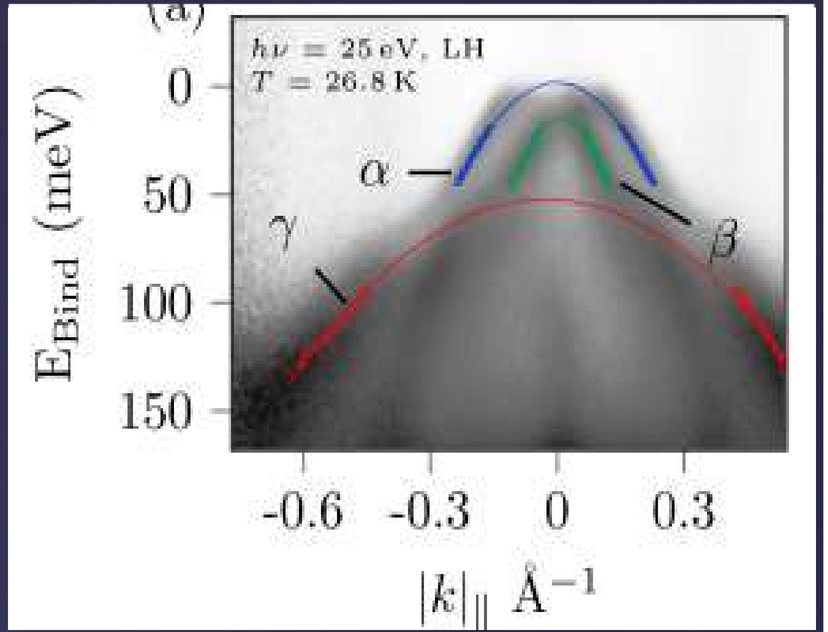


M. D. Watson, AIC,PRB 91, 155106 (2015)

Orbitally-dependent band renormalization of FeSe



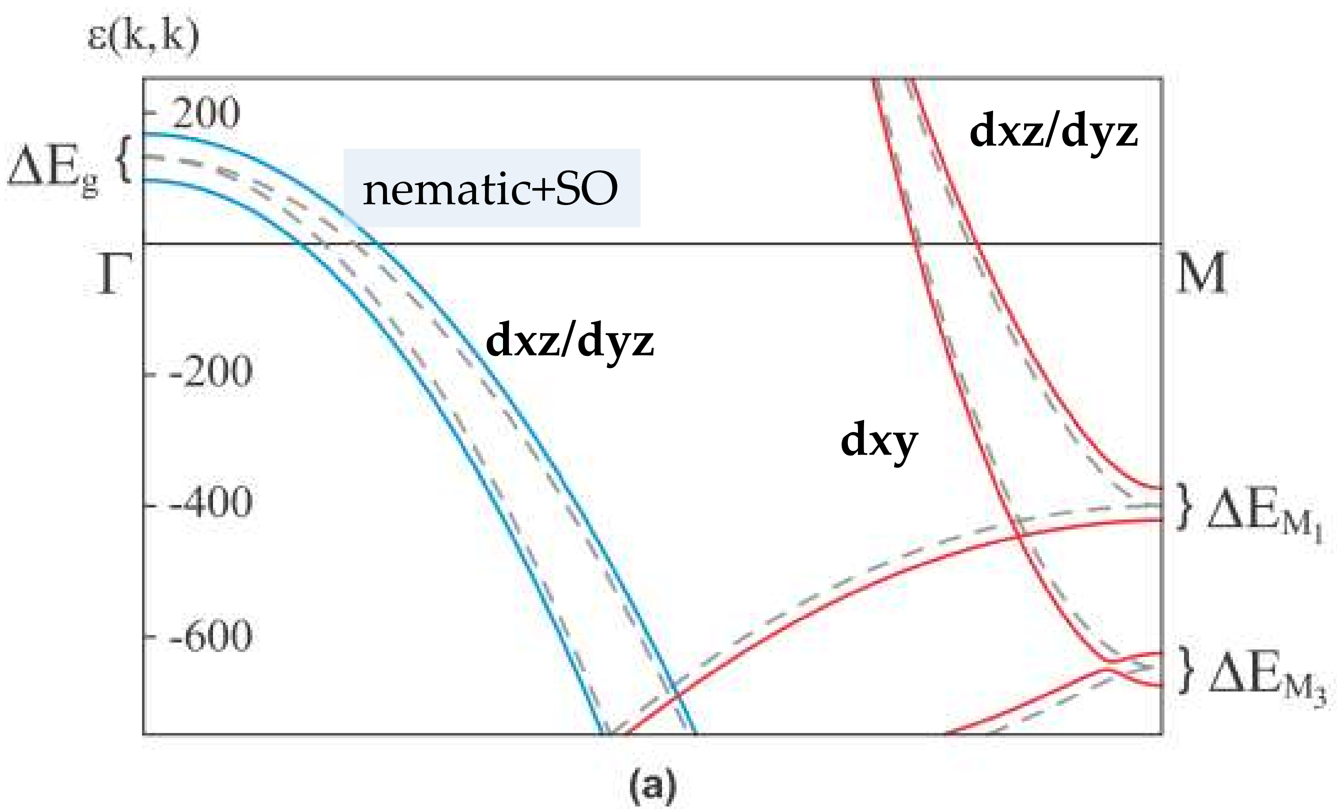


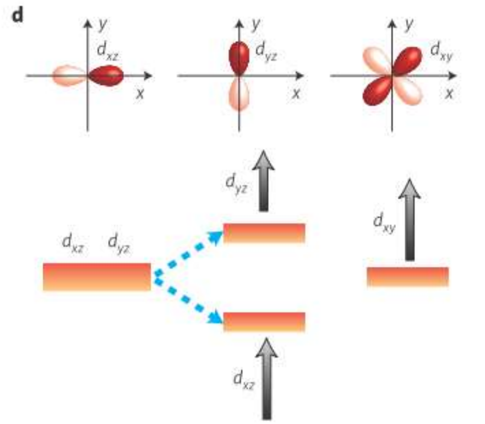


PHYSICAL REVIEW B **89**, 220506(R) (2014)

	α (dxz/dyz)	β (dxz/dyz)	γ dxy	Ref.
FeSe	3.2	2.1	8	Our work
FeSe	3	3.7	9	PRB 89, 220506 (2014)
FeSe0.42Te0.52	1	6	17	PRL 104, 097002 (2010)

Lifting of degeneracy in P4/nmm symmetry group





Nematic-**dxz/dyz** on-site energy anisotropy

dxy (two Fe/unit cell) hopping anisotropy

$$\Delta E_g = \sqrt{\lambda^2 + \varphi_\Gamma^2},$$

$$\Delta E_{M_1} = \varphi_1 - \frac{(\varphi_1 + \varphi_3)\,\lambda^2}{4\,(\epsilon_1 - \epsilon_3)^2} + O(\lambda^2\varphi^3)$$

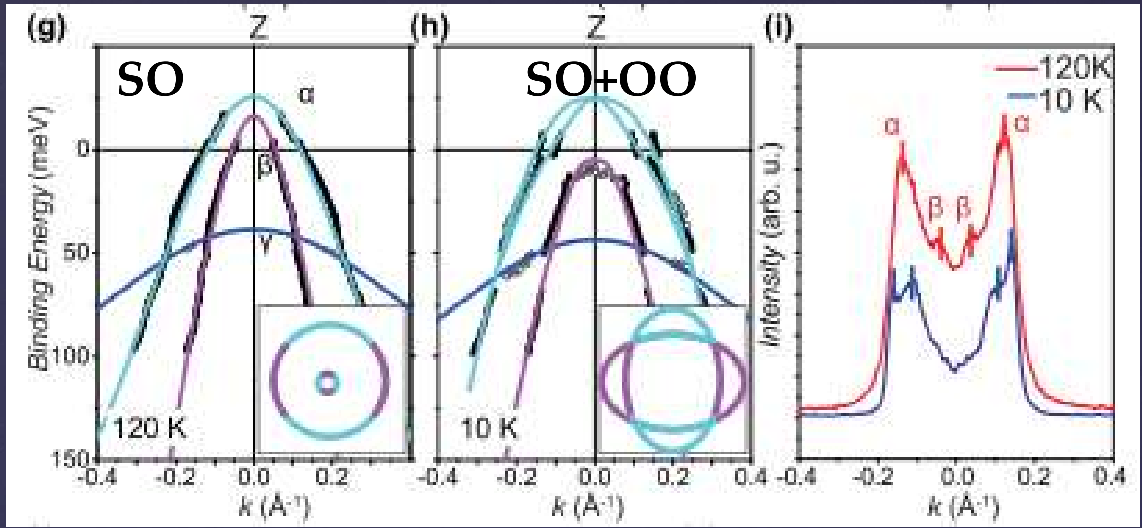
$$\Delta E_{M_3} = \varphi_3 - \frac{(\varphi_1 + \varphi_3)\,\lambda^2}{4\,(\epsilon_1 - \epsilon_3)^2} + O(\lambda^2\varphi^3)$$

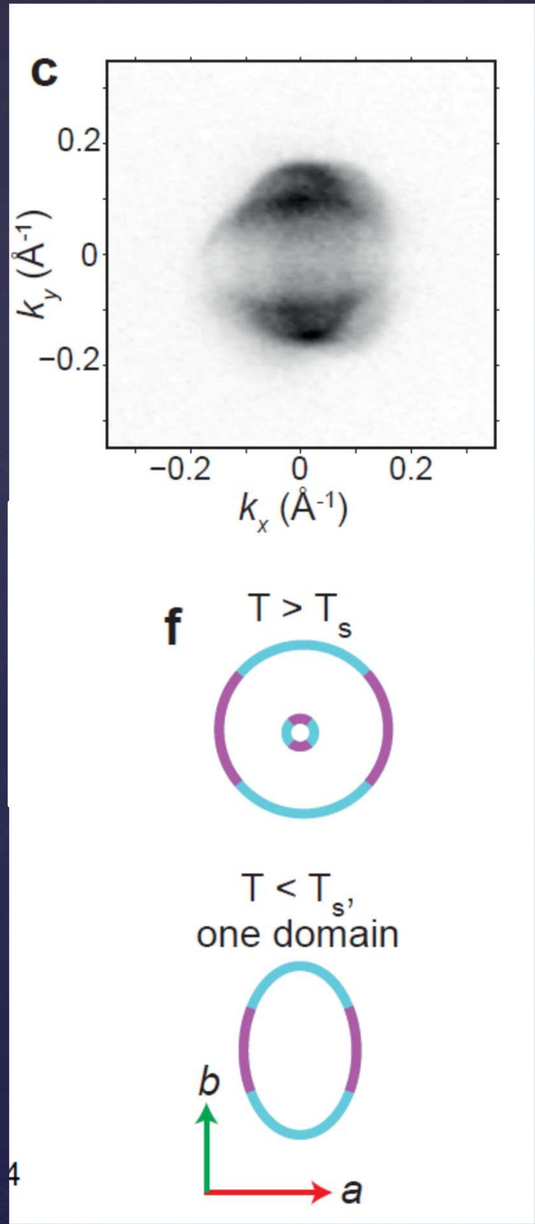
$$H_1 = \frac{\Delta_1}{2}\sum_{\mathbf{k}\sigma}(c^\dagger_{xz,\mathbf{k}\sigma}c_{xz,\mathbf{k}\sigma} - c^\dagger_{yz,\mathbf{k}\sigma}c_{yz,\mathbf{k}\sigma})$$

$$H_3 = \frac{\Delta_3}{2}\sum_{\mathbf{k}\sigma} c^\dagger_{xy(1),\mathbf{k}\sigma}c_{xy(2),\mathbf{k}\sigma}\sin\left(\frac{k_x}{2}\right)\sin\left(\frac{k_y}{2}\right)$$

R. M. Fernandes and O. Vafek, PRB 90, 214514 (2014)

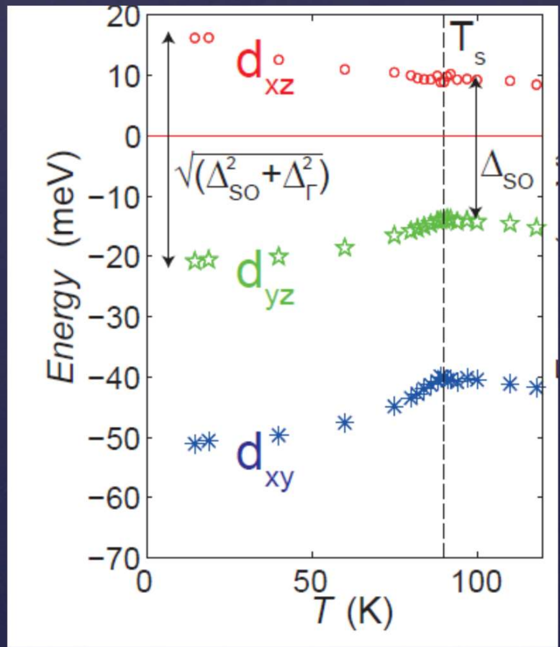
ARPES studies on FeSe: Hole bands





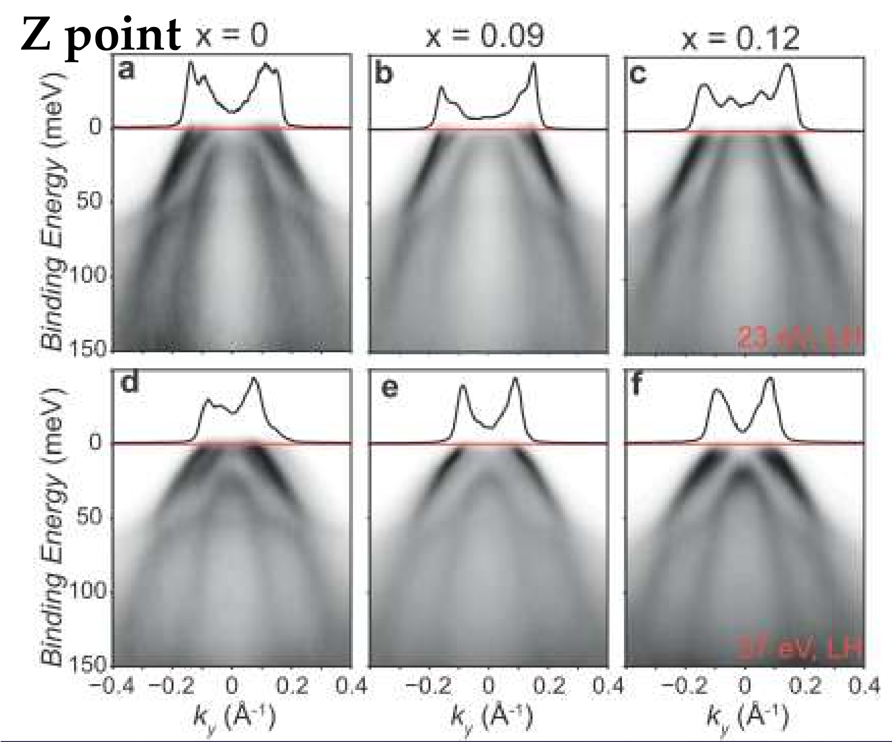
-Spin-orbit coupling around 20 meV;
-Orbital order ~14.5 meV
-Elongation of the hole pocket at low T; d-wave Pomeranchuck instability;

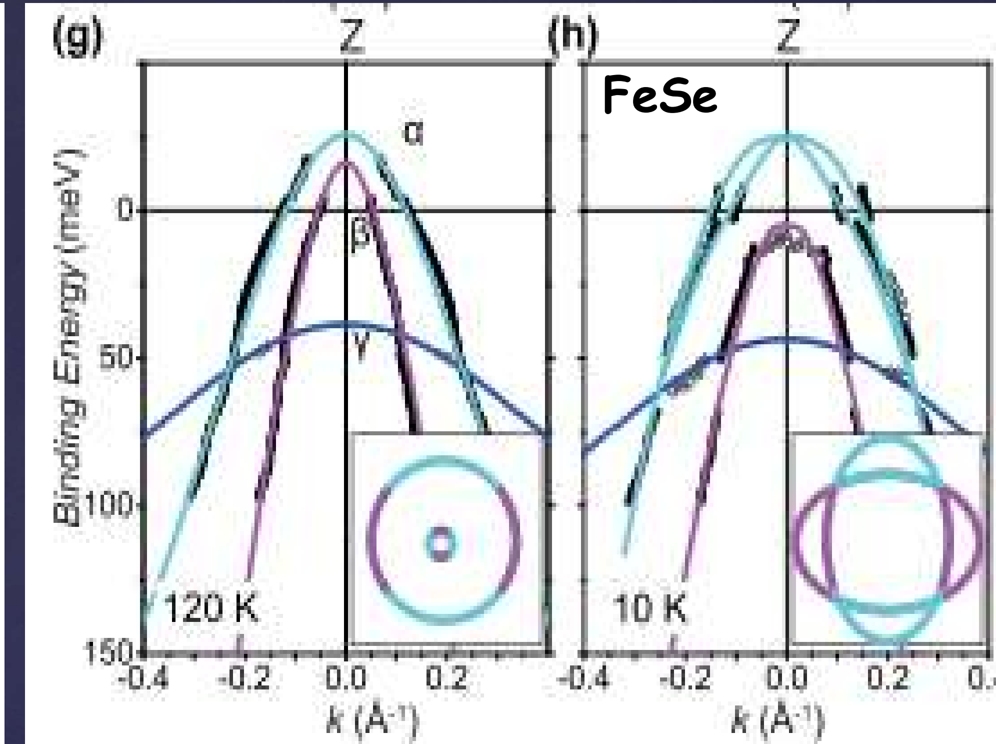
(two ellipses due to the twinning effect);

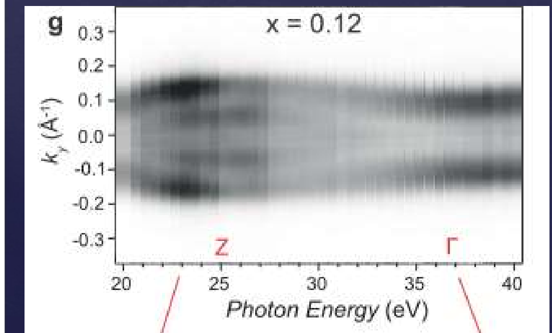


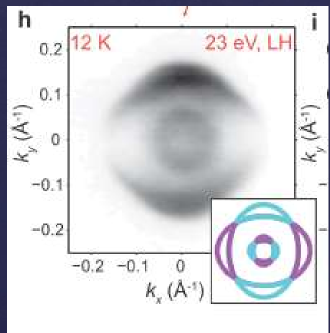
M. D. Watson et al., PRB 91, 155106; J. Phys. Soc. Jpn. 86, 053703 (2017); arXiv.1706.00338

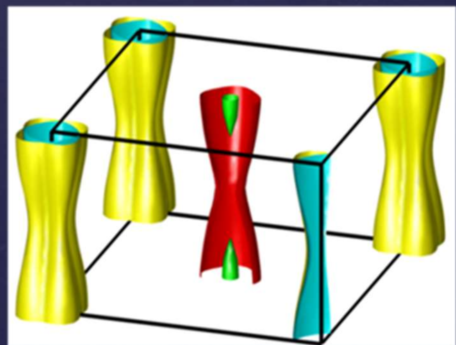
Suppressing orbital order in $Fe(Se_{1-x}S_x)$

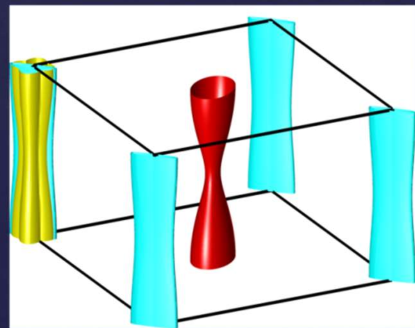






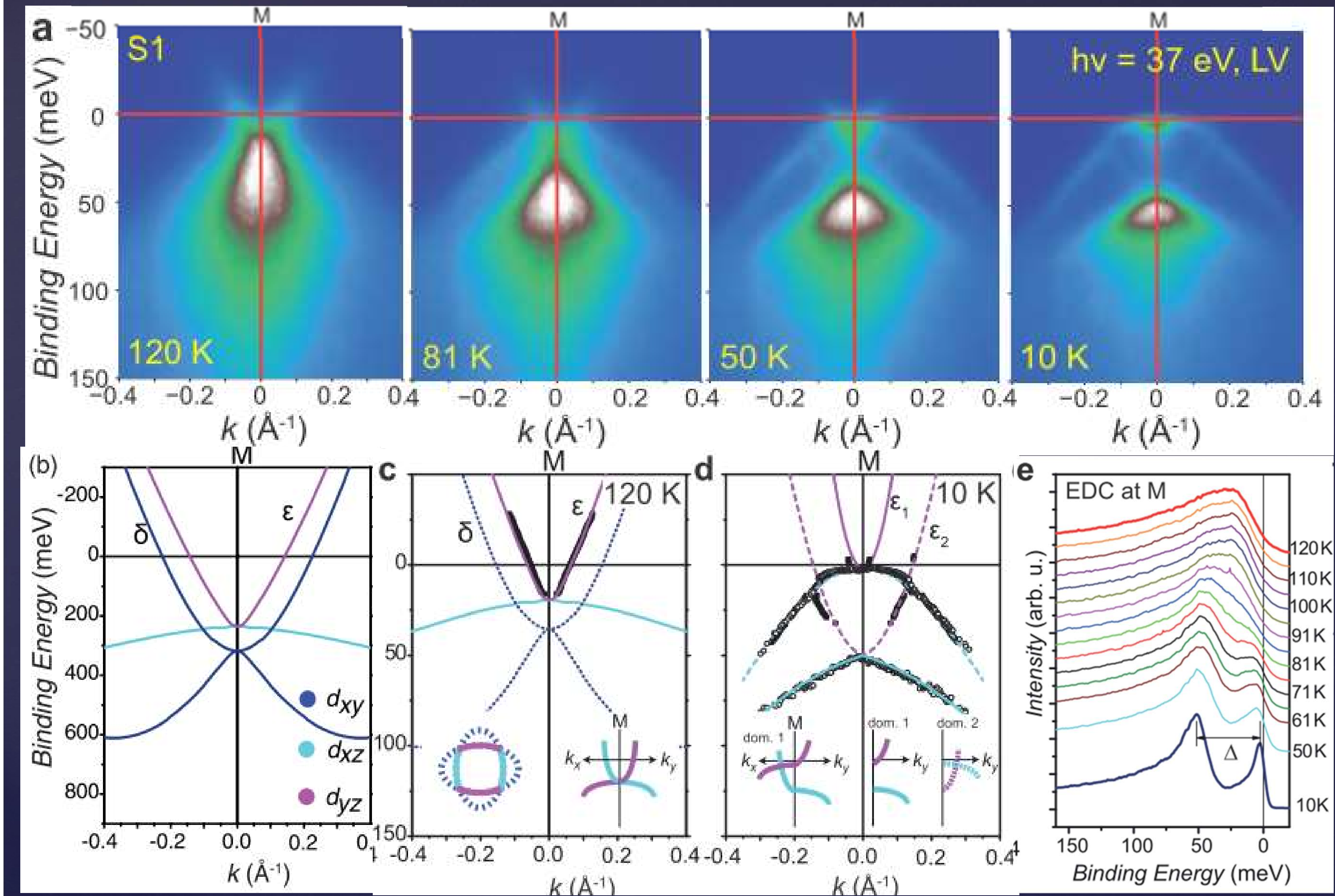






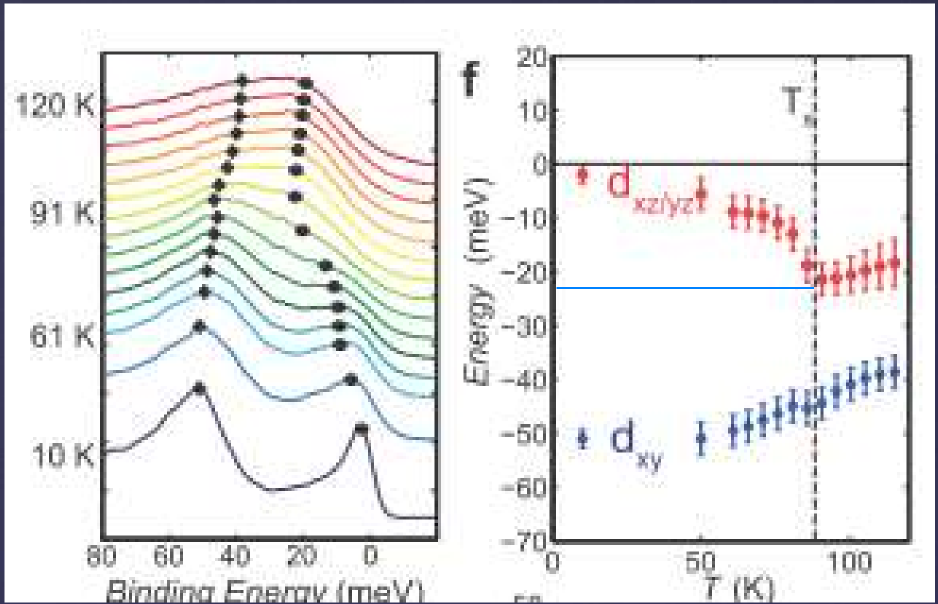
M.D. Watson, AIC, Phys. Rev. B 92, 121108 (2015)

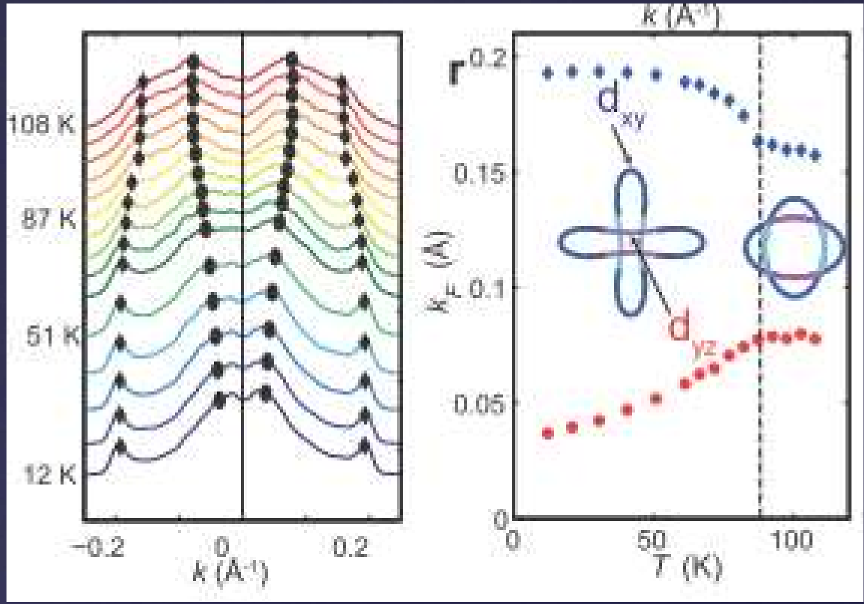
ARPES studies on FeSe: Electron bands

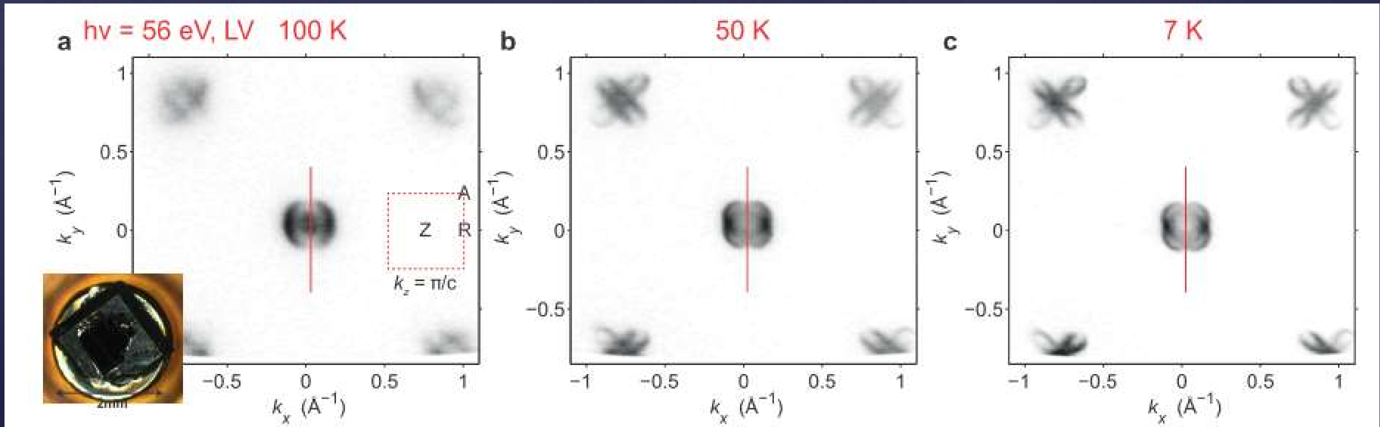


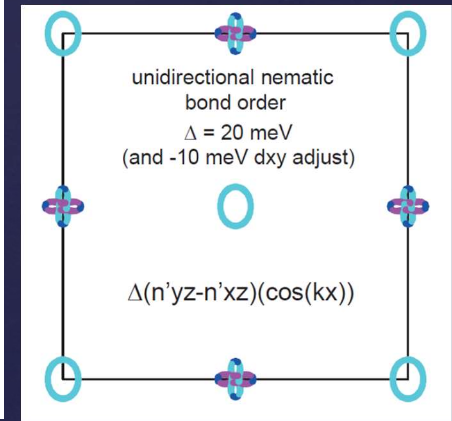
M. D. Watson, AIC, PRB 91, 155106 (2015)

Splitting of the both dxy vs dxz/yz bands at the M point



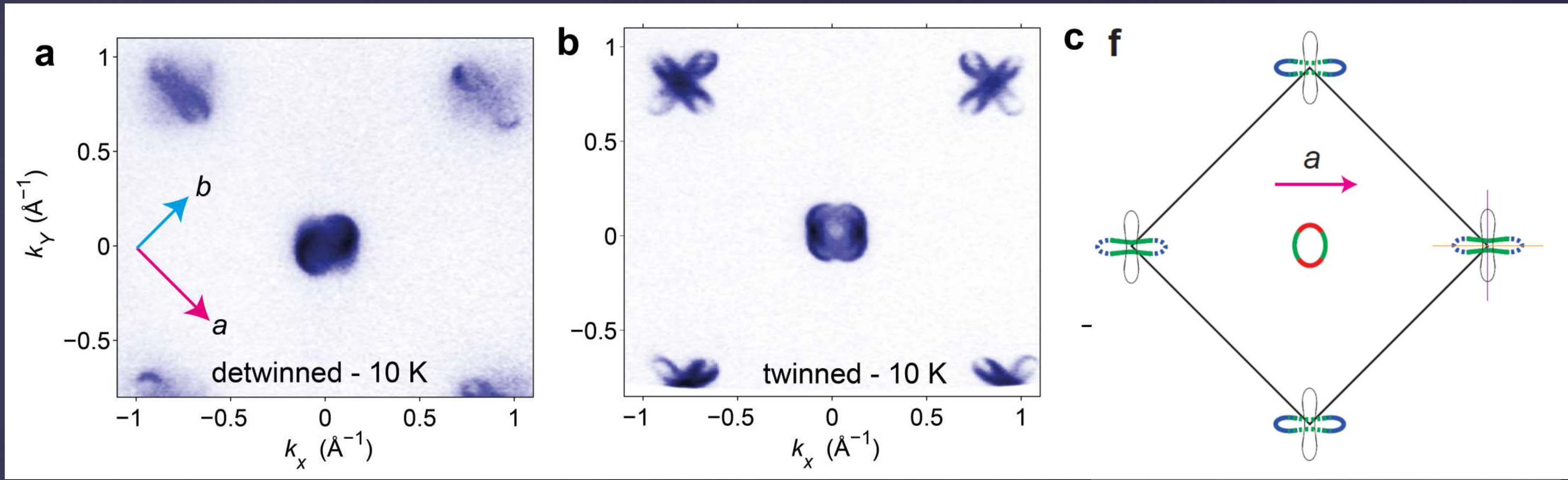


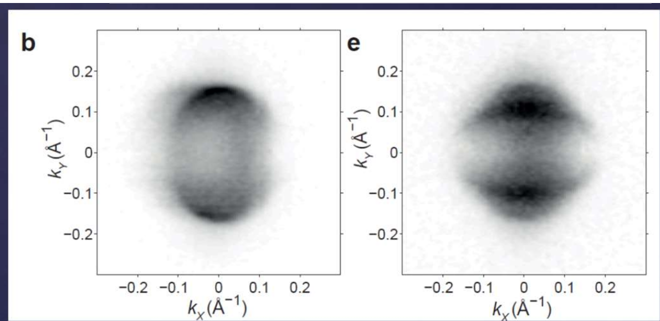




M. Watson et al., PRB 94, 201107 (2016)

Detwinned ARPES measurements of FeSe

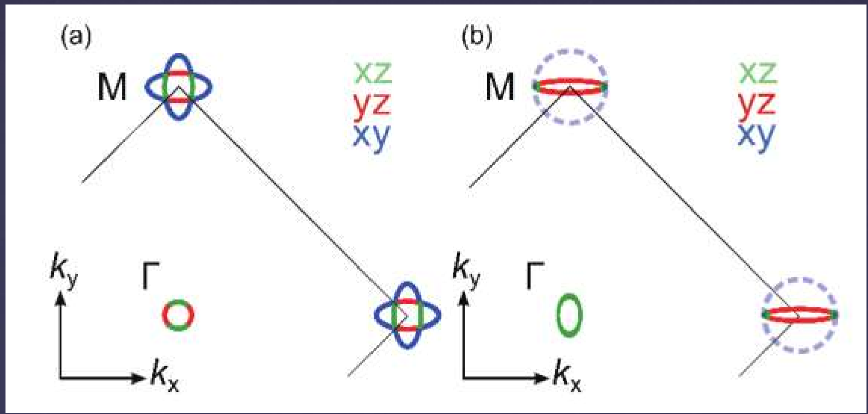




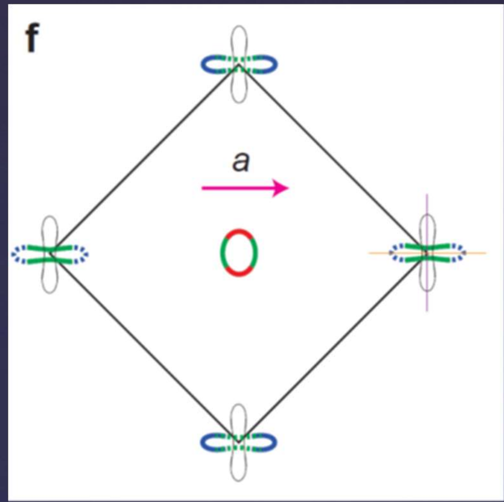
- Strained/detwinned sample, only the peanut-shaped electron pockets along the a axis is observed!
- dxz dispersions are observed; similar renormalization to dyz;

M. Watson et al., arXiv:1705.02286

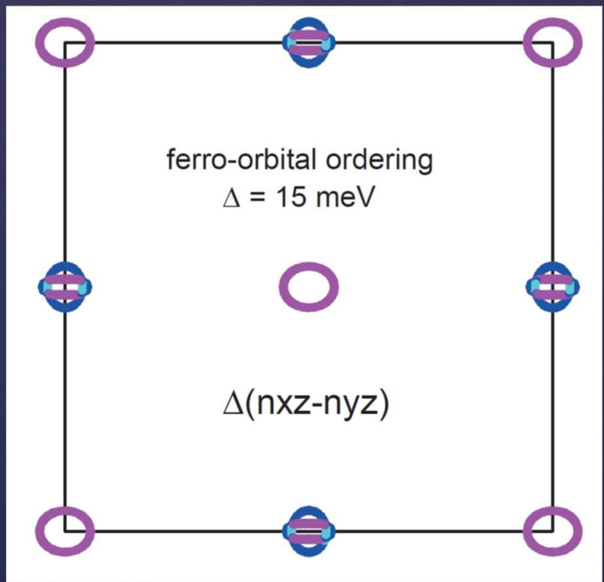
Orbital ordering in FeSe

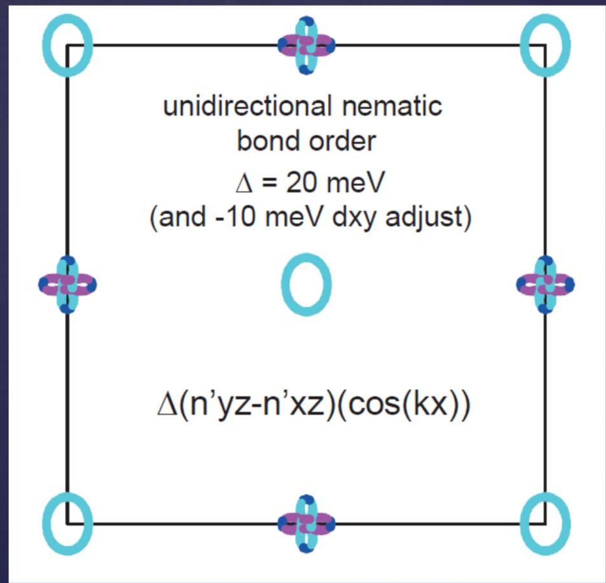


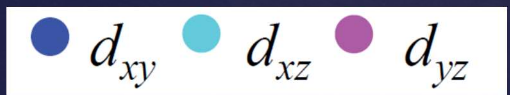
Y. Suzuki et al., arXiv: 1504.00980



M. Watson et al., arXiv:1705.02286

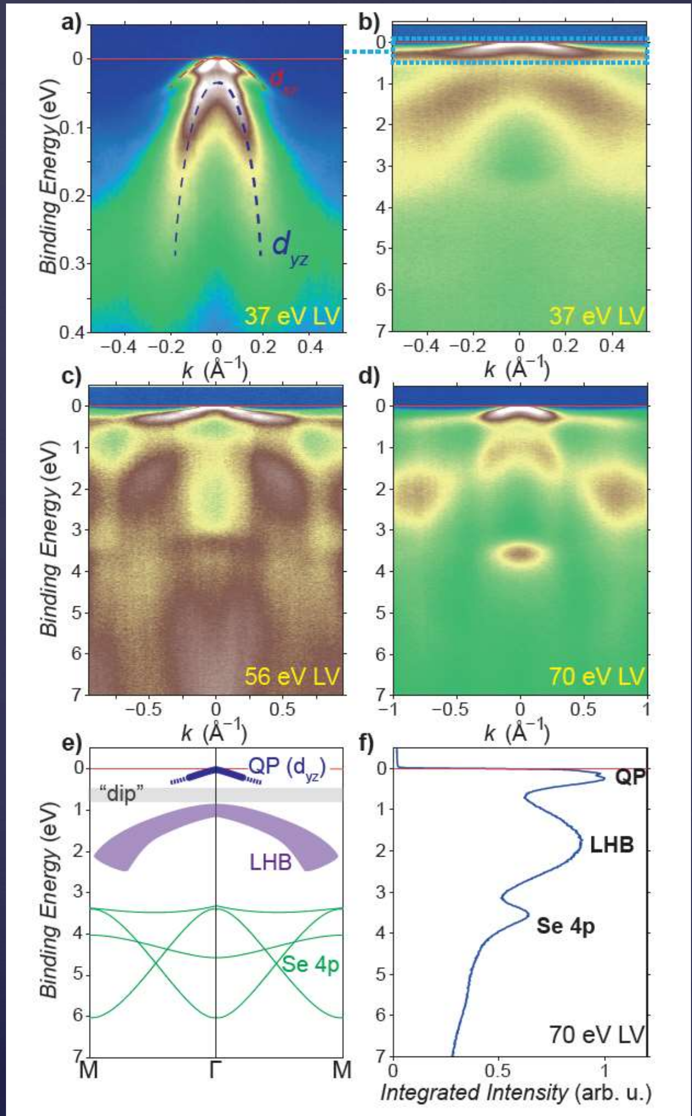


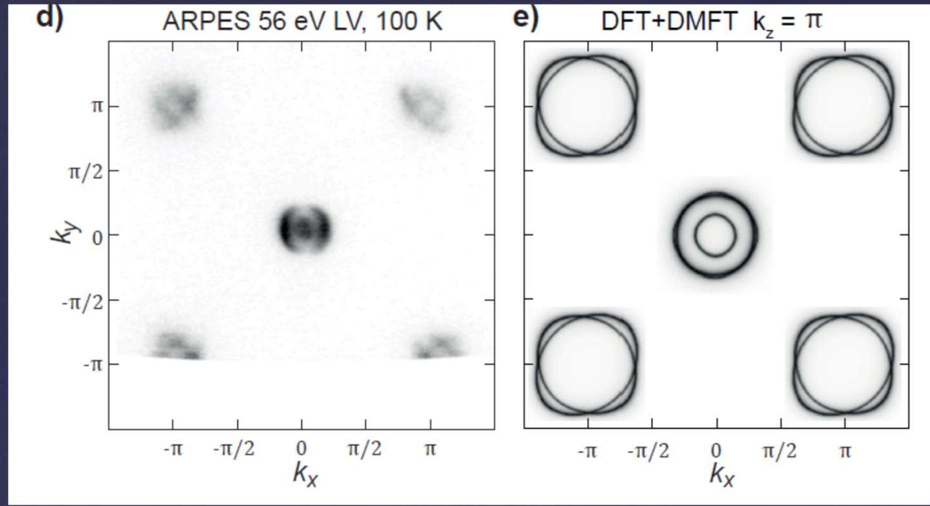


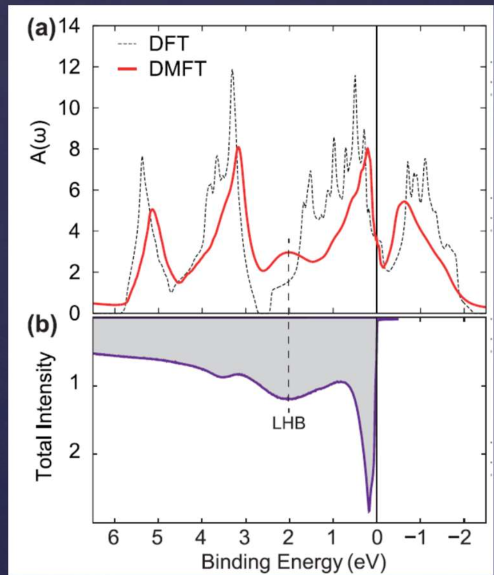


M. Watson et al., PRB 94, 201107 (2016)

Strong correlations in FeSe. Lower Hubbard band



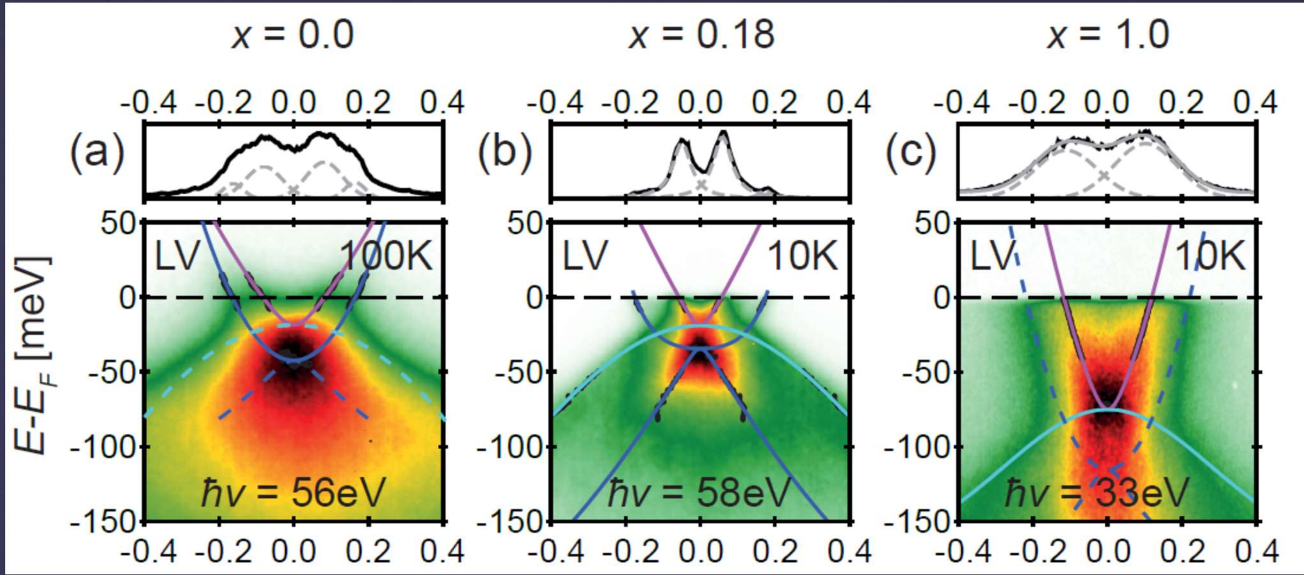


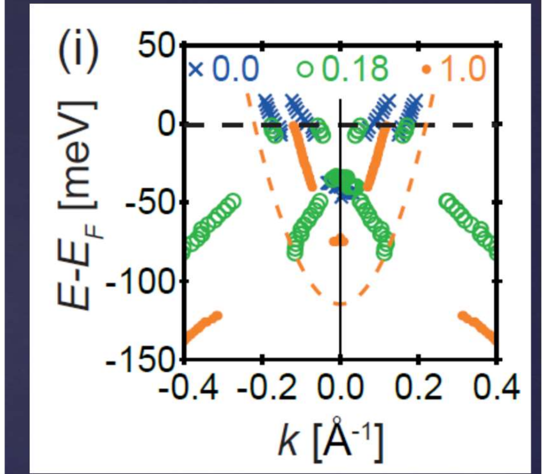


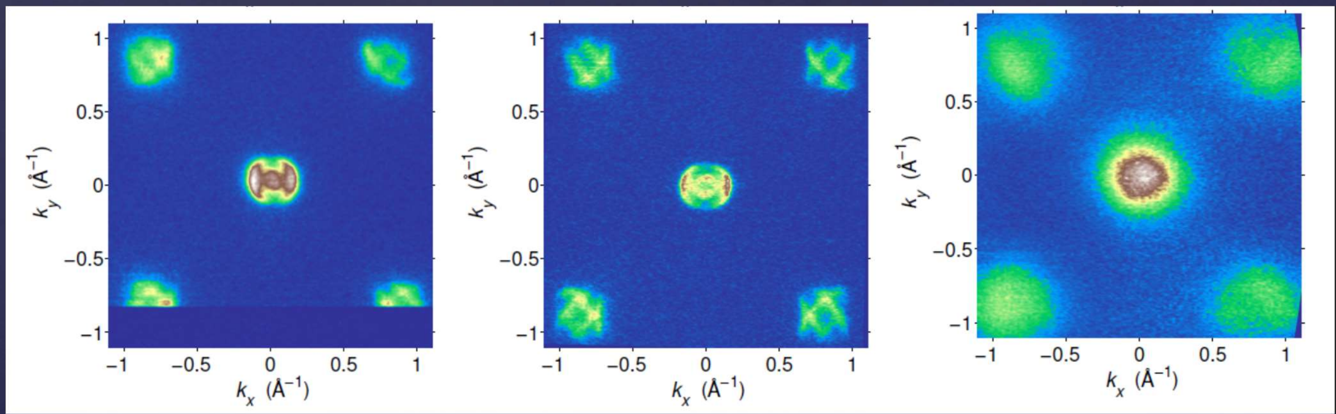
U=4 eV,
J_H=0.8 eV

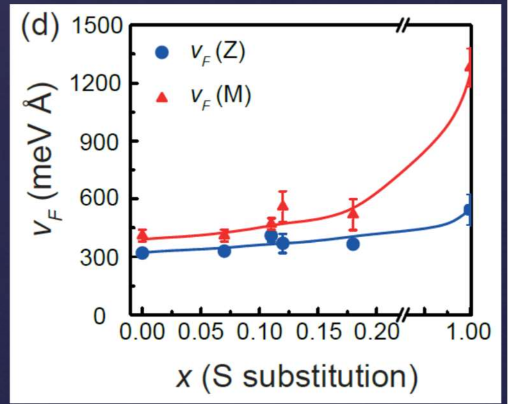
M.D. Watson et al., PRB 95, 081106 (2017)
(collaboration with R. Valenti)

Suppressing electronic correlations in $Fe(Se_{1-x}S_x)$





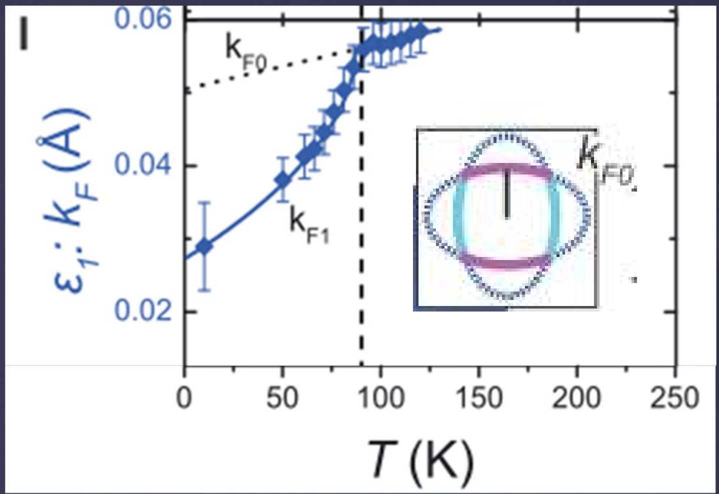


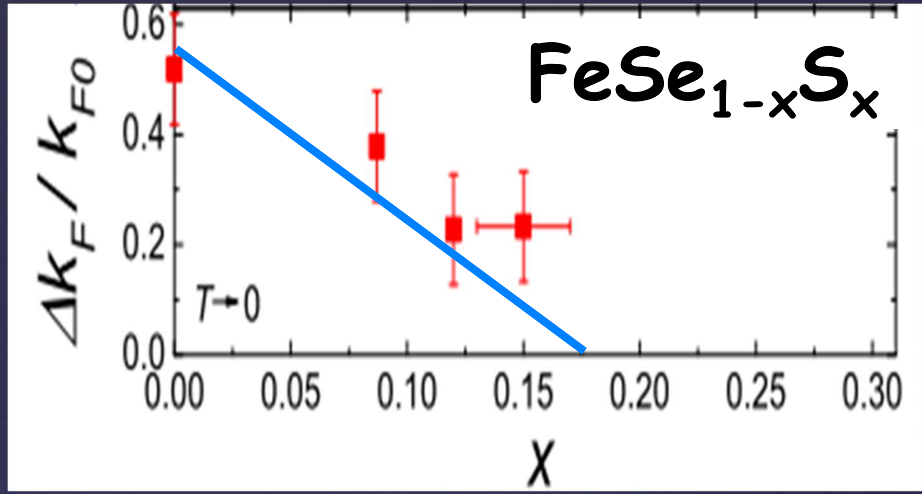


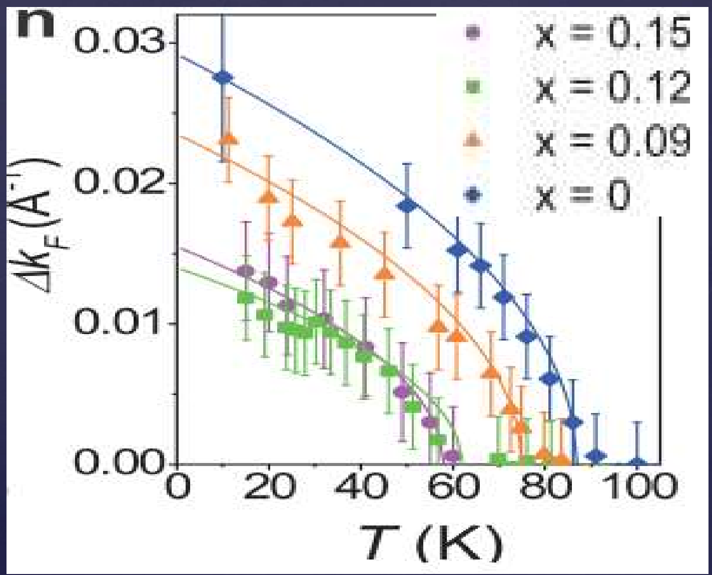
P. Reiss et al. AIC , arXiv:1705.11139

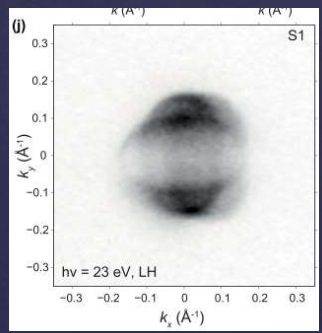
Tetragonal phases

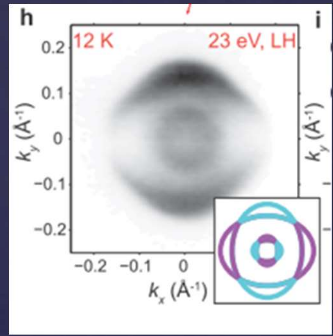
Fermi surface deformation in the nematic phase

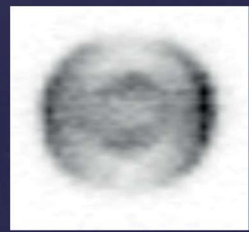












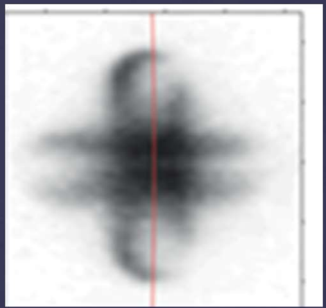
X=0

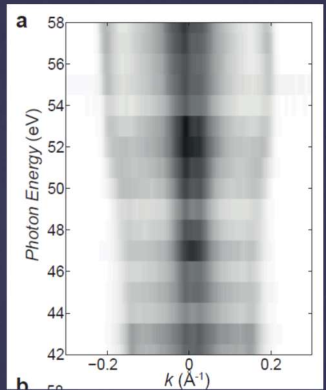
X=0.12

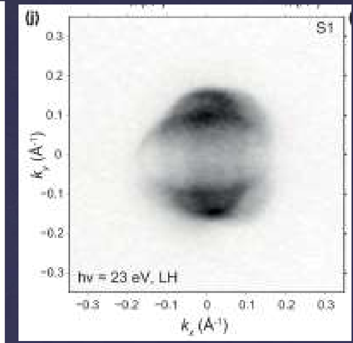
X=0.18

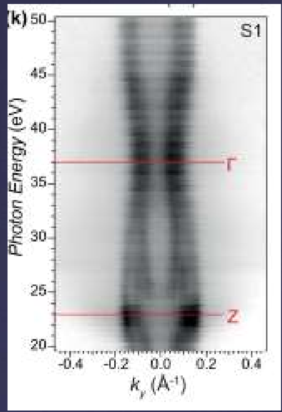
M.D. Watson, AIC, Phys. Rev. B 92, 121108 (2015); PRB 91, 155106 (2015)[
P. Reiss et al. AIC , arXiv:1705.11139

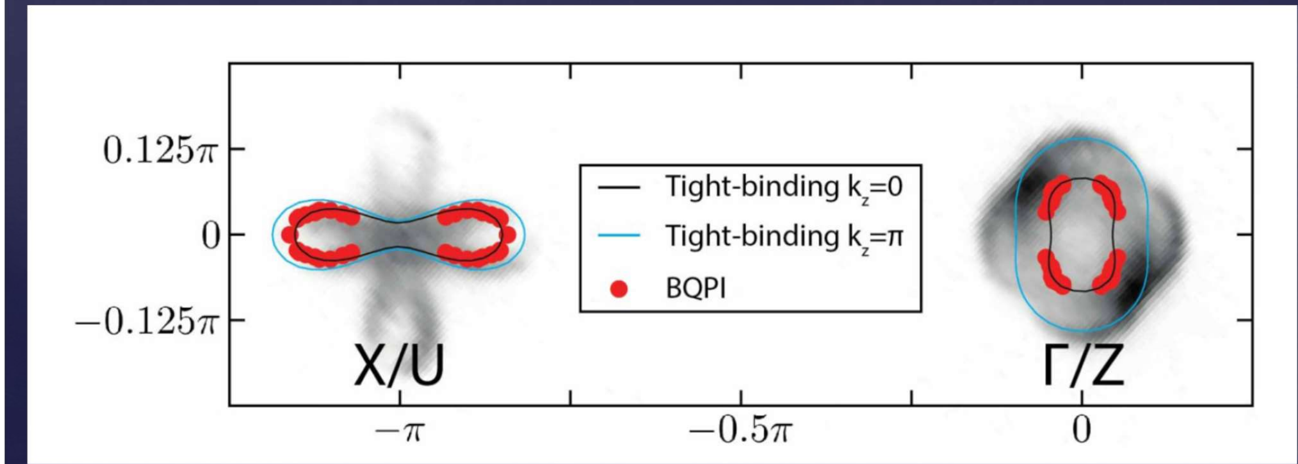
Anisotropic superconducting gap. Orbitally-selective Cooper pairing in FeSe

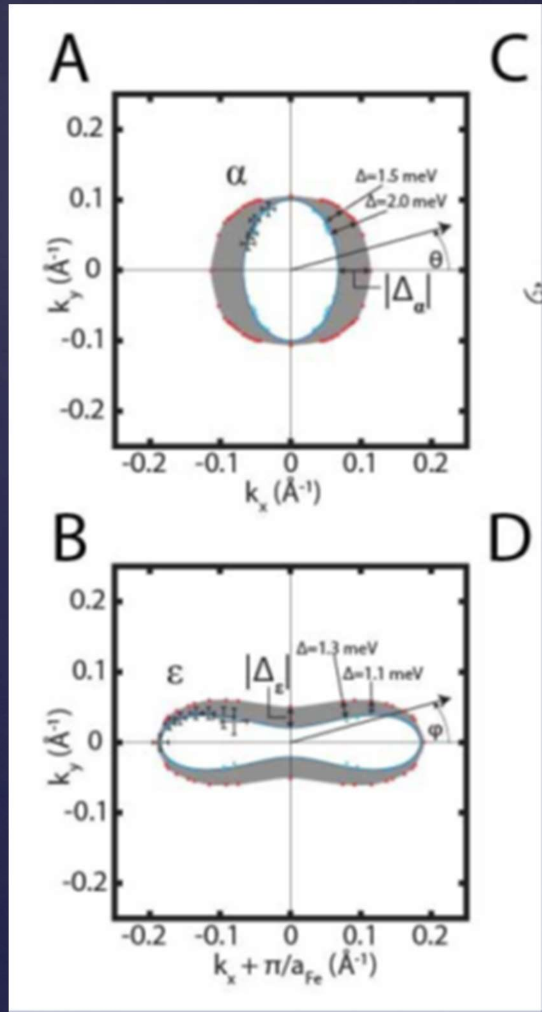










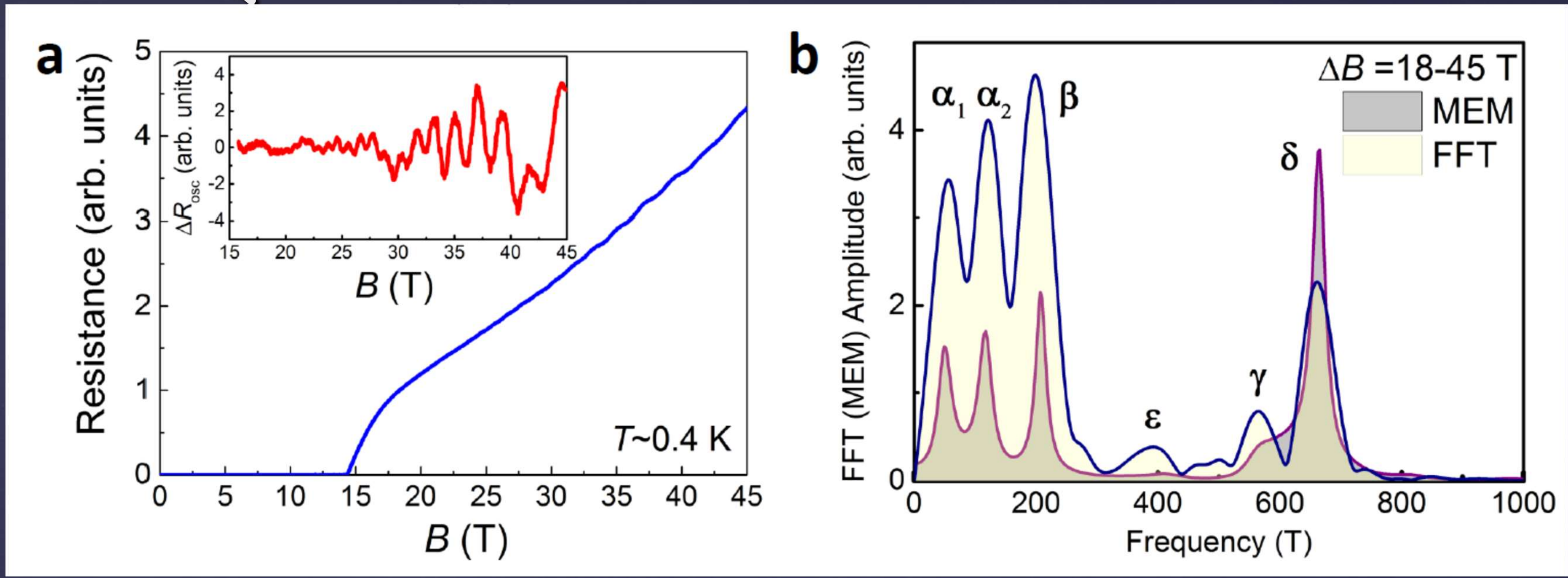


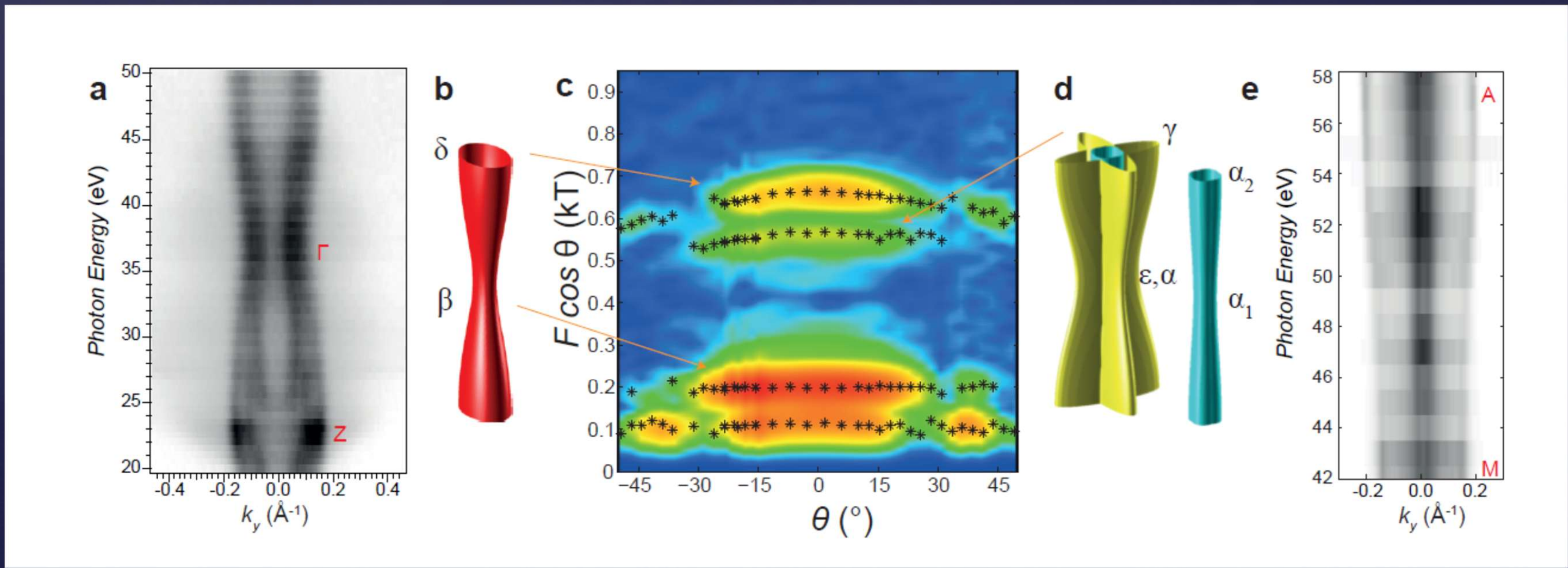
P. O. Sprau et al., Science 357, 75 (2017)

III. Quantum oscillations in $Fe(Se_{1-x}S_x)$

M. D. Watson, AIC,PRB 91, 155106 (2015); PRL. 115, 027006 (2015);
AIC et al. arXiv:1611.07424;

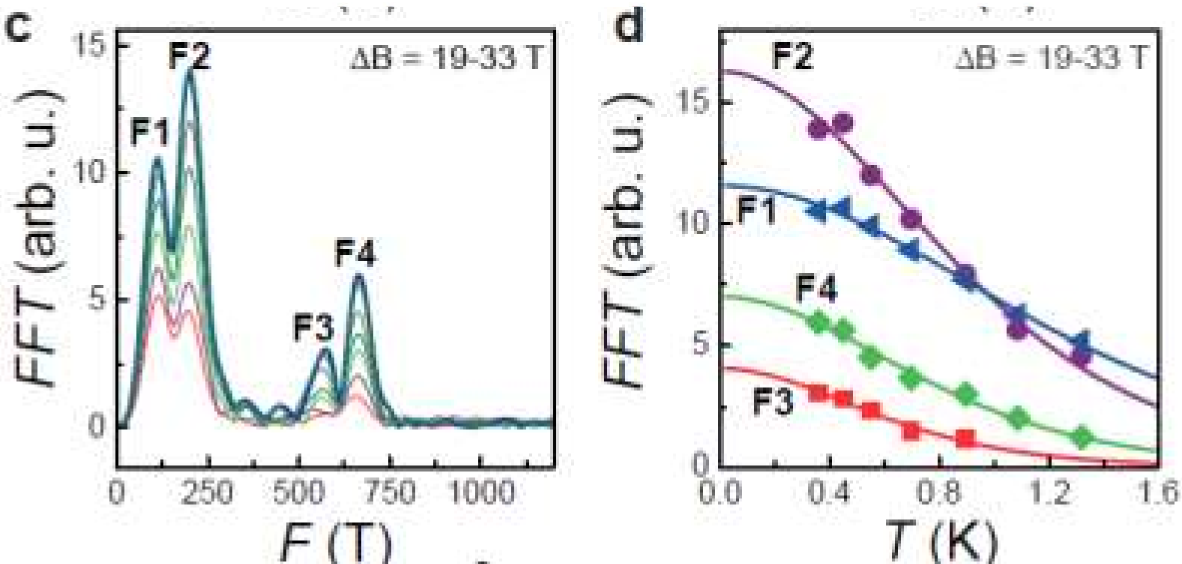
Quantum oscillations in FeSe





Quantum oscillations in FeSe

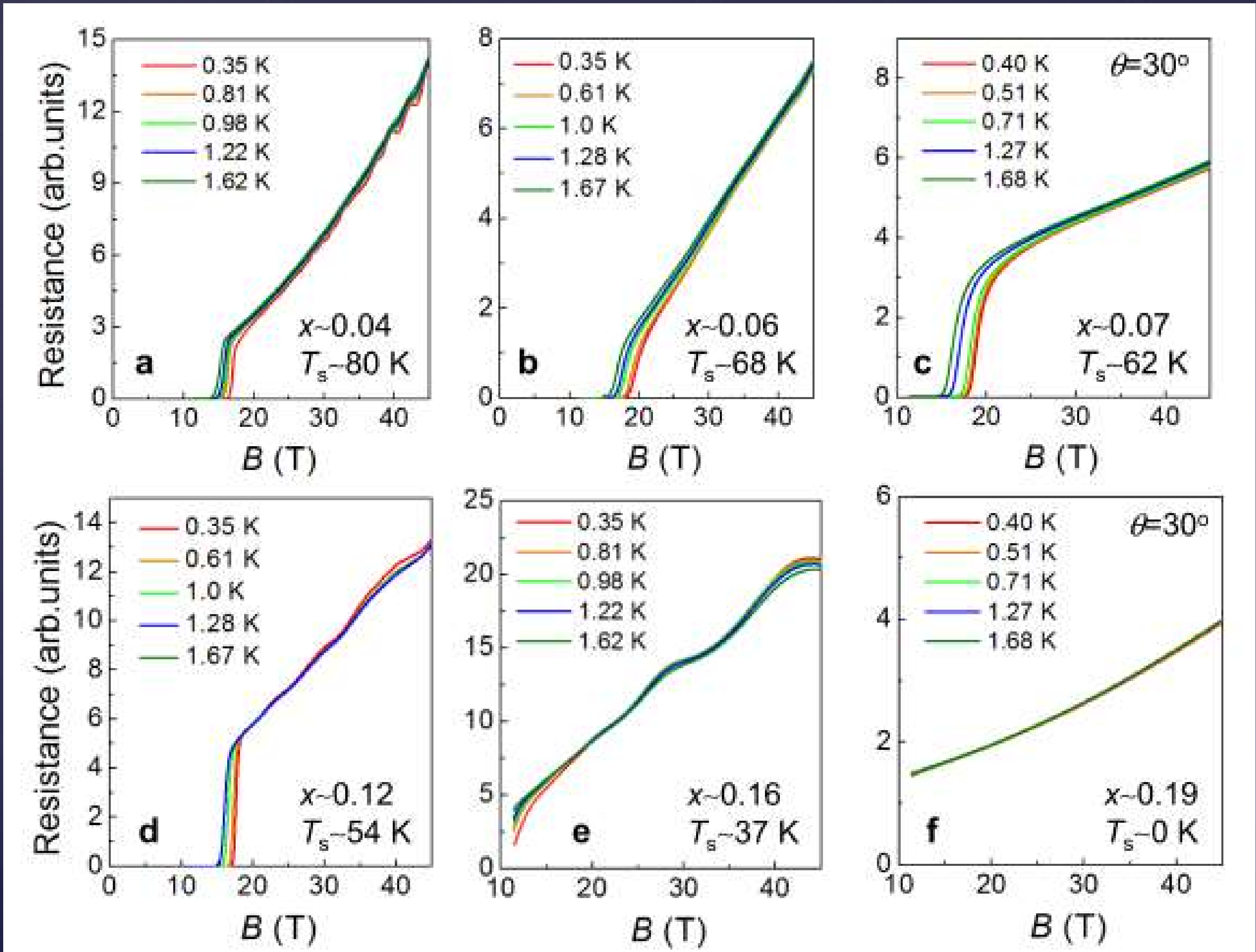
Branch	F (kT)	m^*/m_e	A (%BZ)	k_F (Å^{-1})	E_F (meV)
α	0.06	1.9(2)	0.20	0.043	3.6
β	0.20	4.3(1)	0.69	0.078	5.4
γ	0.57	7.2(2)	2.0	0.13	9.1
δ	0.68	4.2(2)	2.3	0.14	18



	F (T)	m* (m_e)
F1	114	3.0(5)
F2	200	4.1(5)
F3	568	6(1)
F4	664	4.7(5)

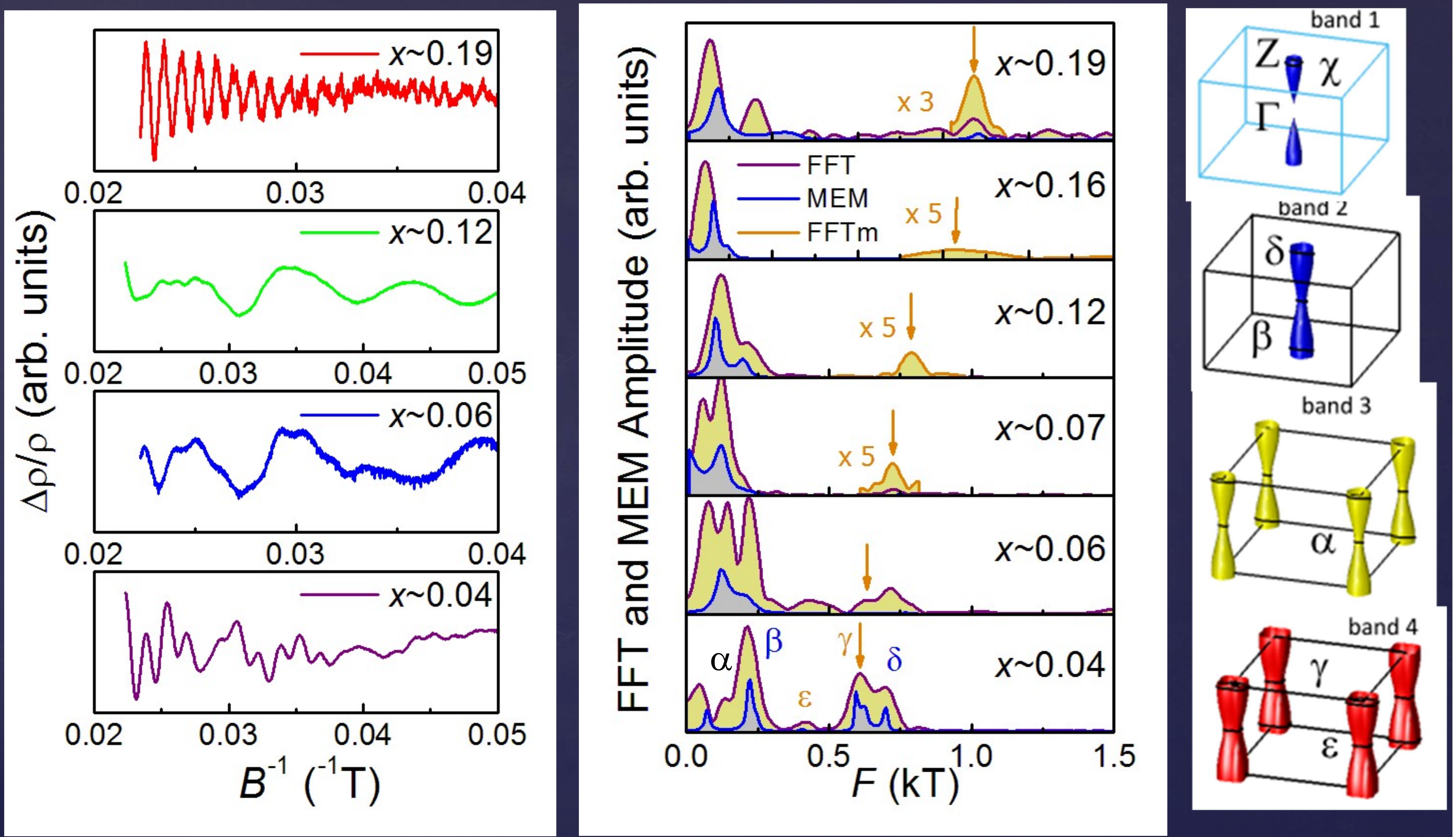
M. D. Watson, AIC,PRB 91, 155106 (2015), T. Terashima et al., PRB 90, 144517

Evolution of the Fermi surface in $Fe(Se_{1-x}S_x)$



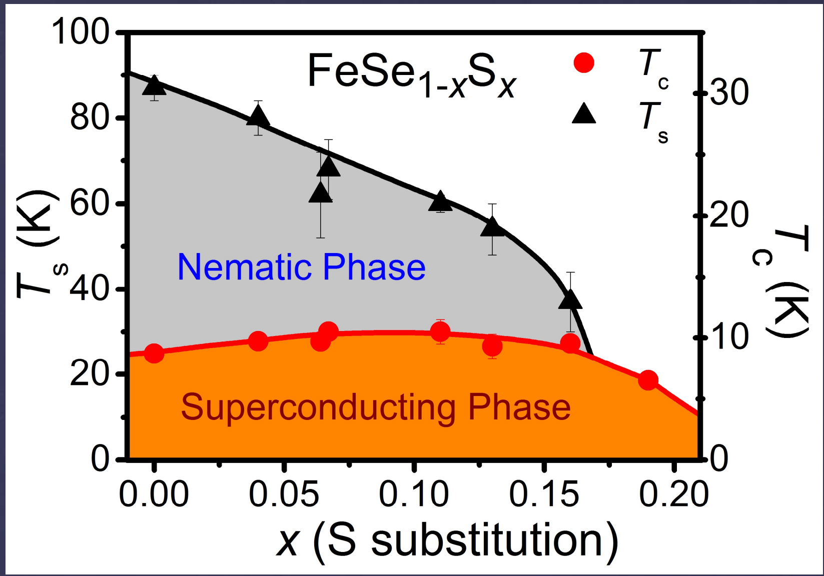
AIC et al., **arXiv:1611.07424**

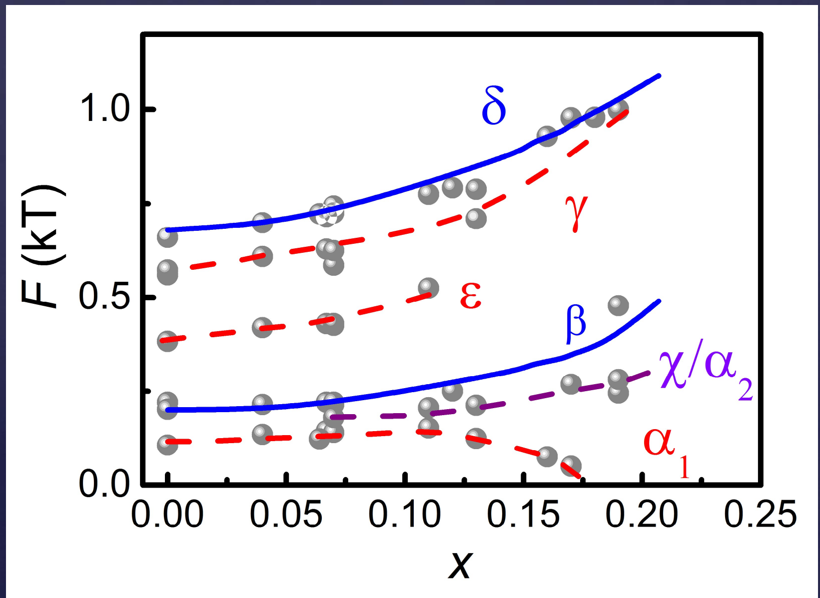
Evolution of the Fermi surface in $Fe(Se_{1-x}S_x)$

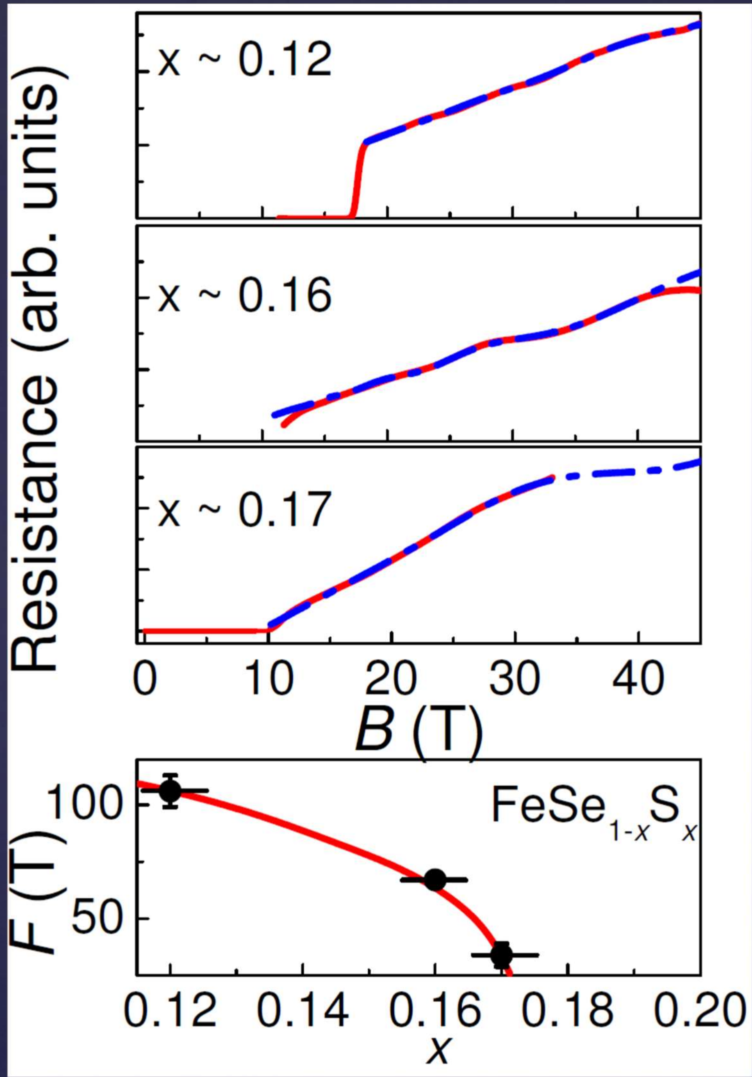


AIC et al., **arXiv:1611.07424**

Fermi surface increase and the Lifshitz transition

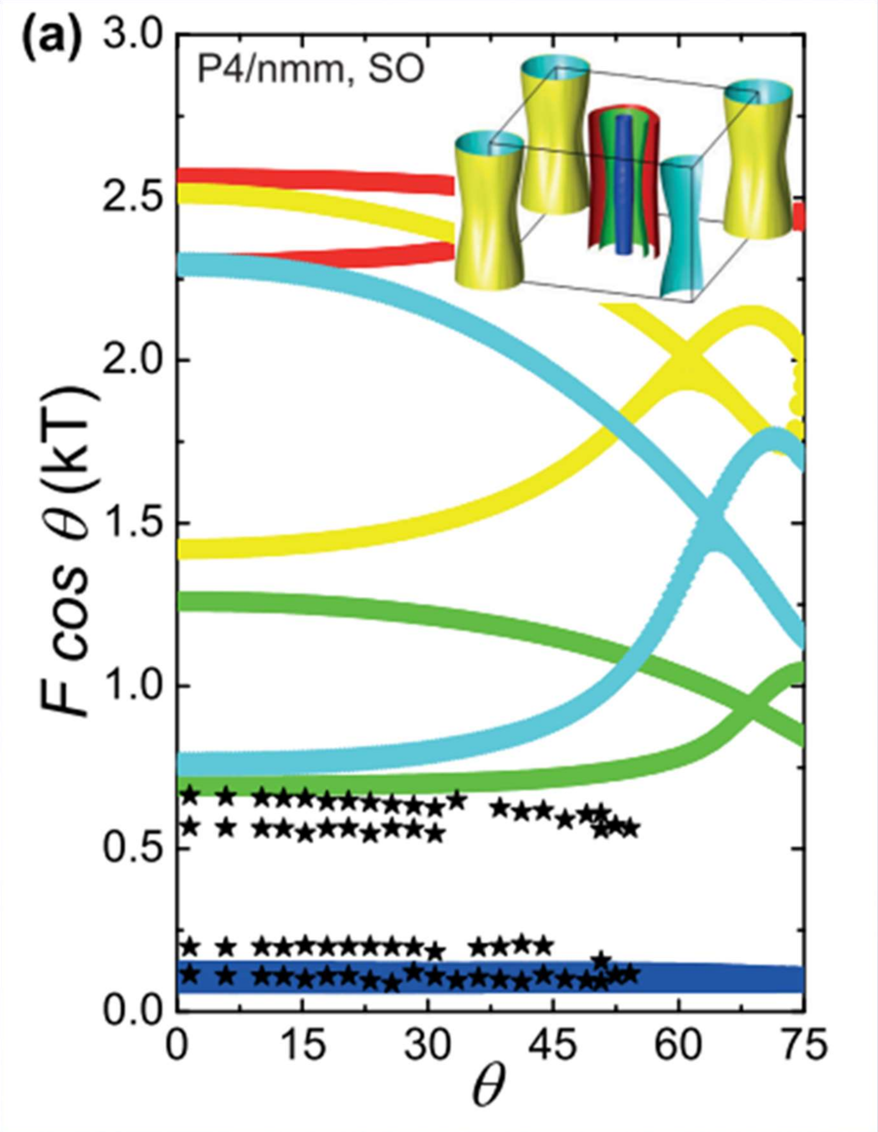


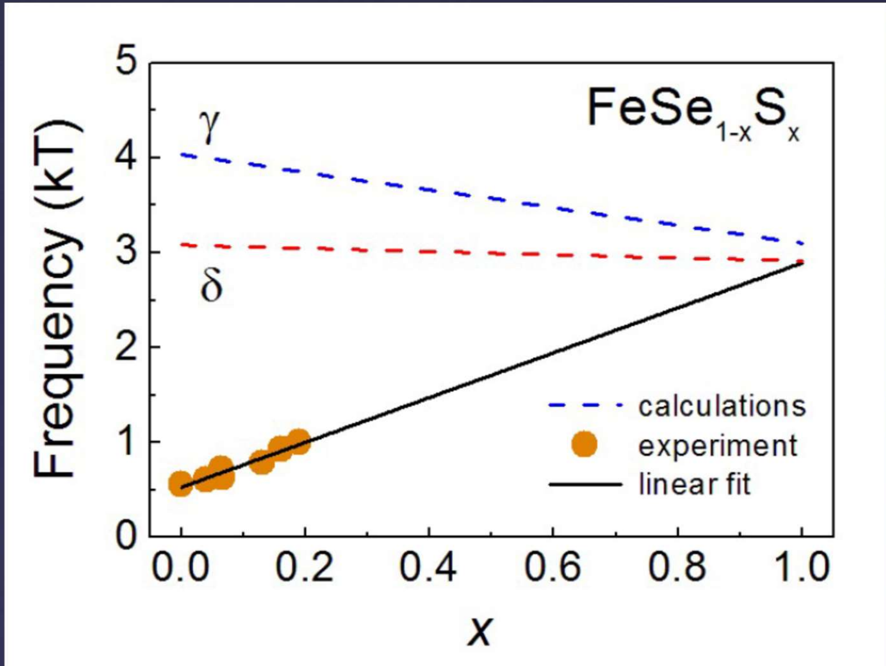


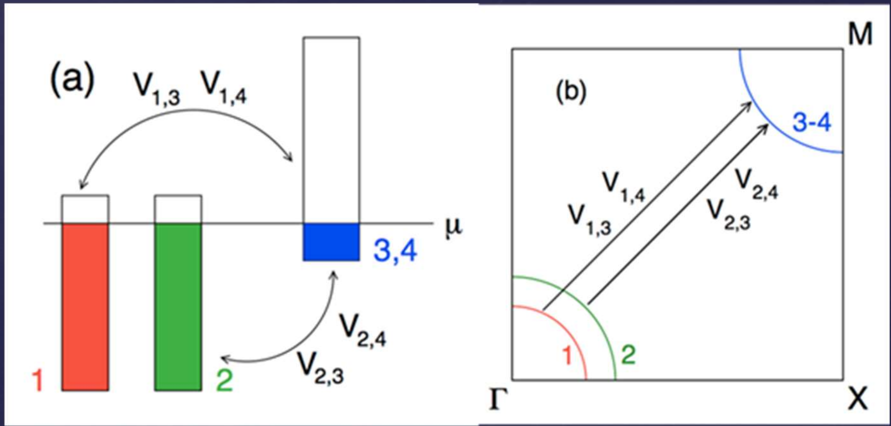


AIC et al., arXiv:1611.07424

Fermi surface shrinking of $Fe(Se_{1-x}S_x)$

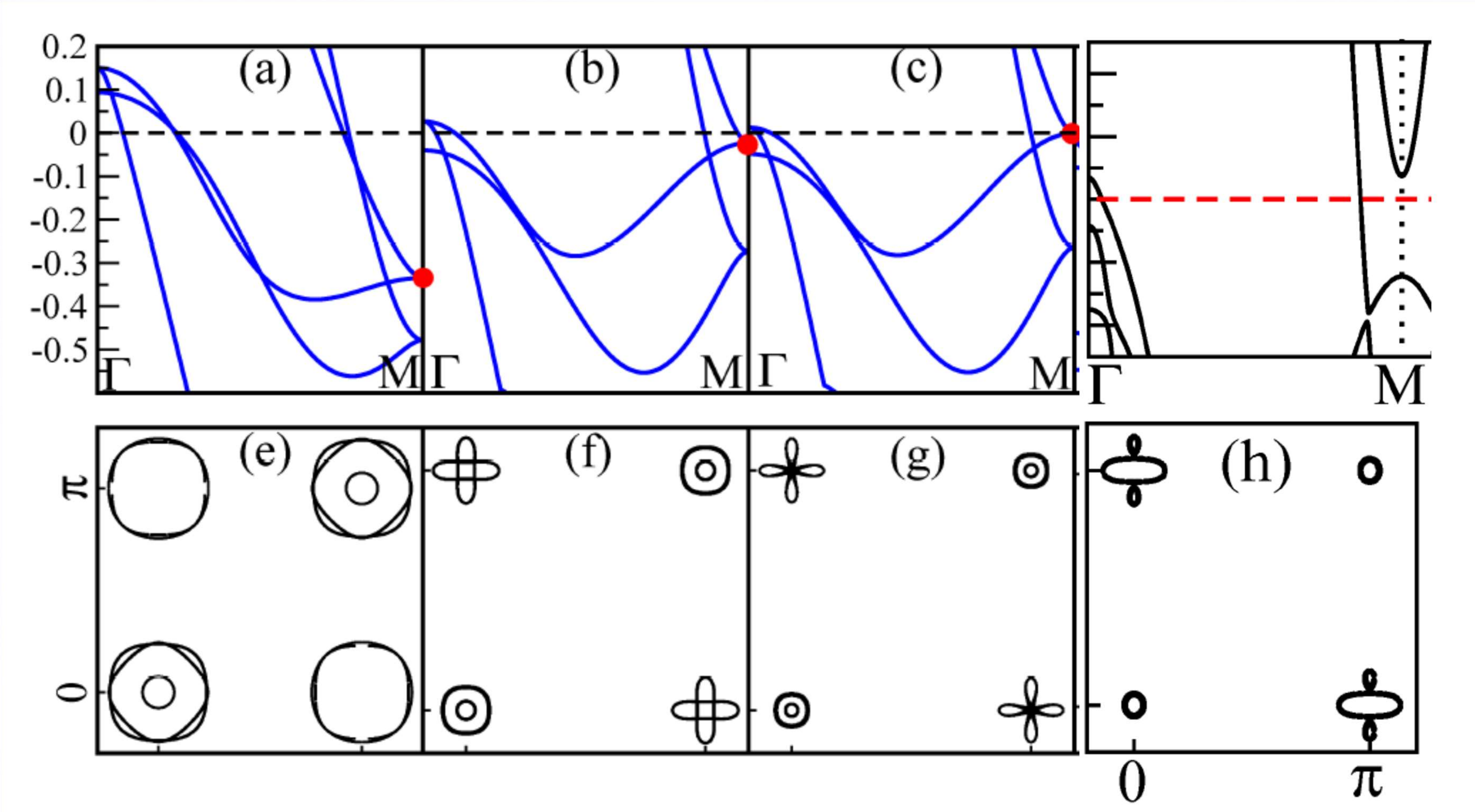






L. Ortenzi *et al.*, PRL 103, 046404 (2009); L. Fanfarillo et al., Phys. Rev. B 94, 155138 (201

The effect of interatomic Coulomb interactions V



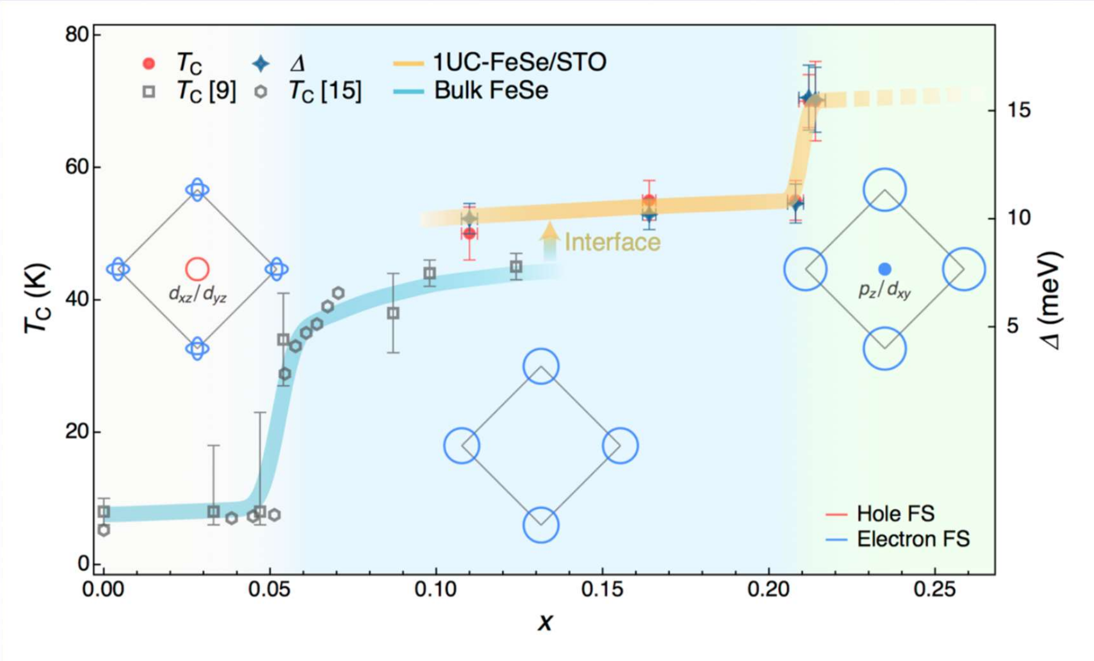
$V = 0$

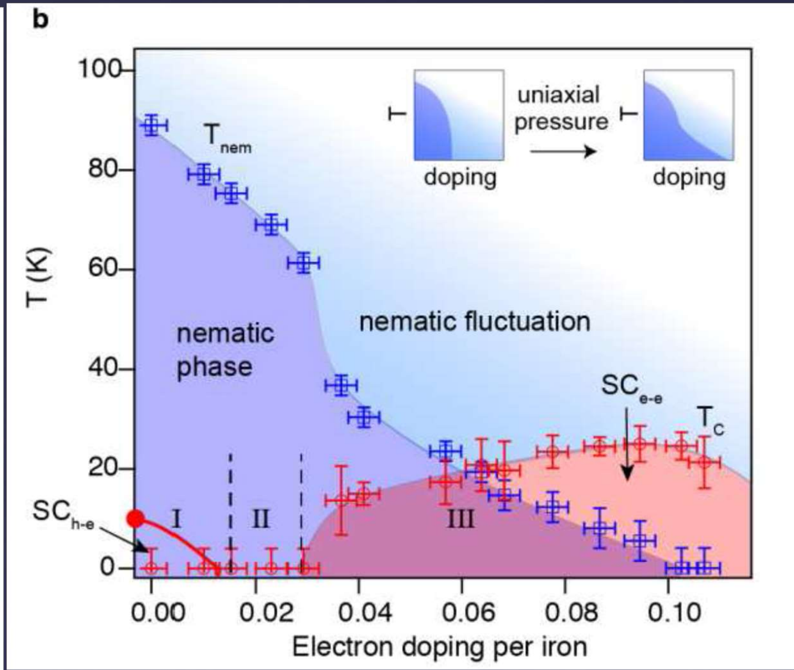
$V = 0.763\text{eV}$

$\lambda_{\text{soc}} = 28\text{meV}$

Kun Jiang et al, Phys. Rev. B 93, 115138 (2016)

Lifshitz transitions in FeSe/STO and K-doped FeSe



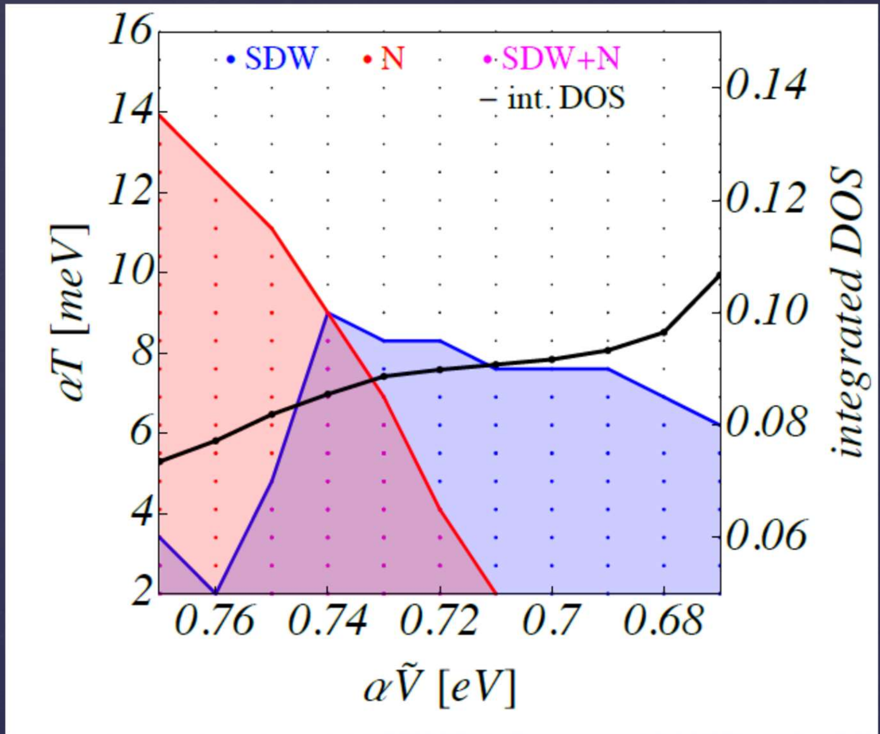


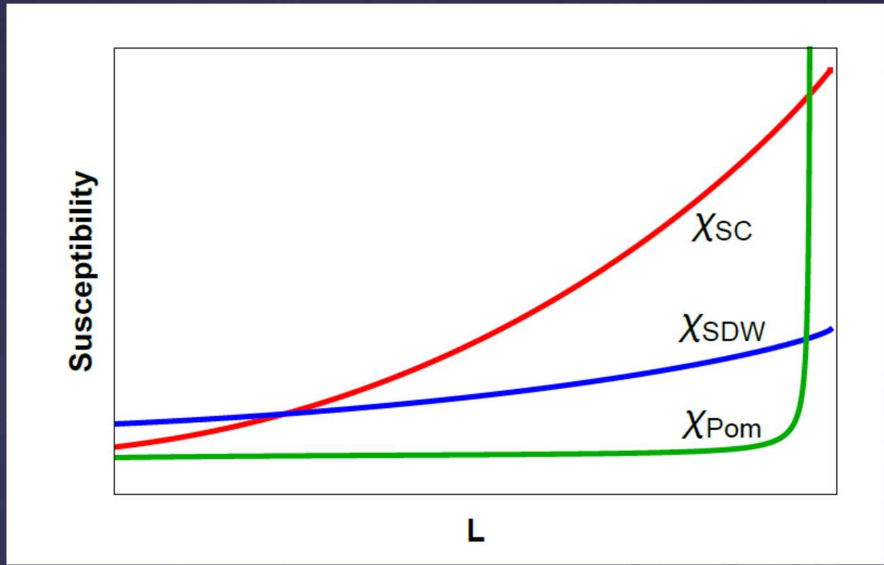
X. Shi, et al., Nat. Comm. 8, 14988 (2017)

Z. R. Ye et al., **arXiv:1512.02526**

Competing and intertwined orders in FeSe

$\alpha U = 1.40$ eV $\quad \alpha J = 0.350$ eV

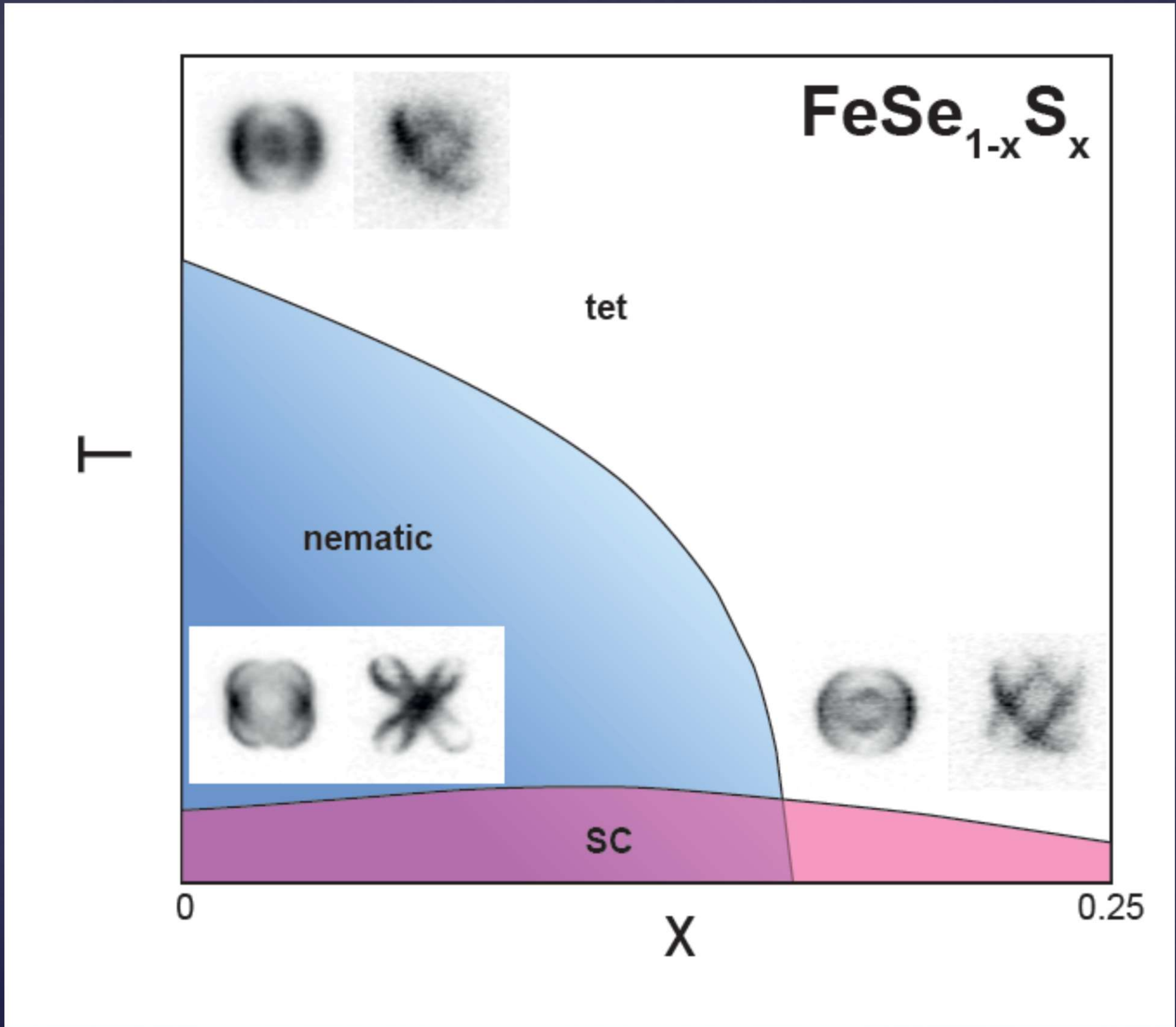




Reduction of inter-site Coulomb interactions → Increase in bandwidth W →

Daniel D. Scherer et al., arXiv: 1612.06085; Rui-Qi Xing et al., arXiv 1611.03912

Key ingredients of the electronic structure of FeSe



Δ_{SO} ~ 20 meV

$\Delta_{u,\Gamma} \approx 14.5$ meV

$\Delta_{u,M} \approx 20$ meV

Lower Hubbard Band
Sizable electronic correlations

U=4 eV,
J_H=0.8 eV

-Small Fermi surfaces
3 bands FeSe
4 bands from x=0.12
Lifshitz transition

- Possible switch for two different SC mechanism

Coldea &Watson, arXiv.1706.00338