New Developments in the Theory of STM on Unconventional Superconductors

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P. Choubey, *et al.*, Phys. Rev. B **90**, 134520 (2014)
A. Kreisel, *et al.*, Phys. Rev. Lett. **114**, 217002 (2015)
A. Kreisel, *et al.,* Phys. Rev. B **94**, 224518 (2016)

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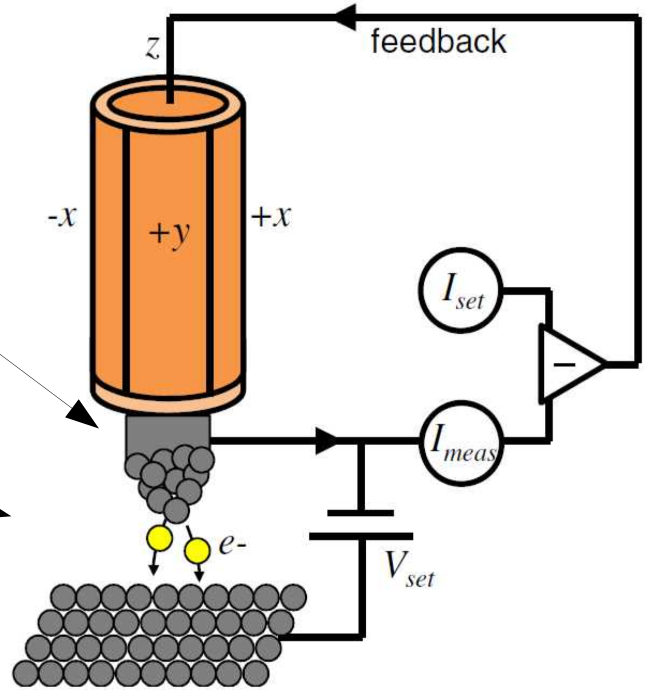
Outline

- Motivation
  - STM: impurities as probe for electronic structure, order parameter and more
  - layered superconductors, complications
- Theoretical methods to investigate impurity physics in superconductors
  - using wavefunction information in layered superconductors: Wannier method
  - Applications
    - LiFeAs (multiband, s-wave)
    - Cuprates: $Bi_2Sr_2CaCu_2O_8$, $Ca_2CuO_2Cl_2$
- Inelastic tunneling
- Bogolibov quasiparticle interference

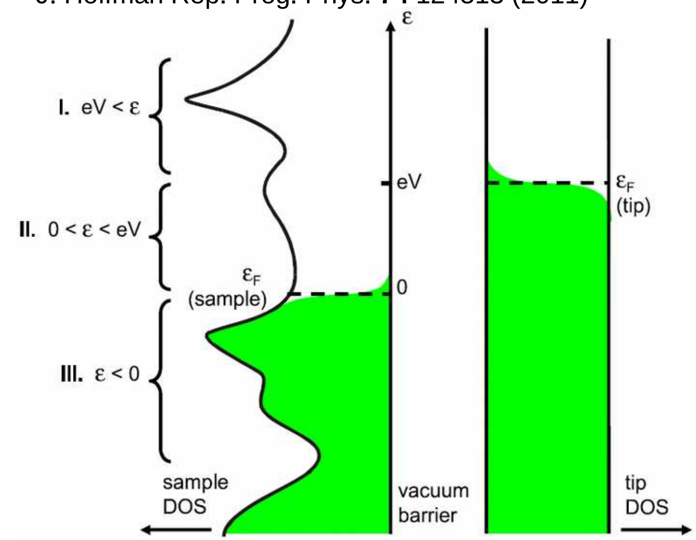
Scanning tunneling microscopy

STM tip

sample e.g. SC



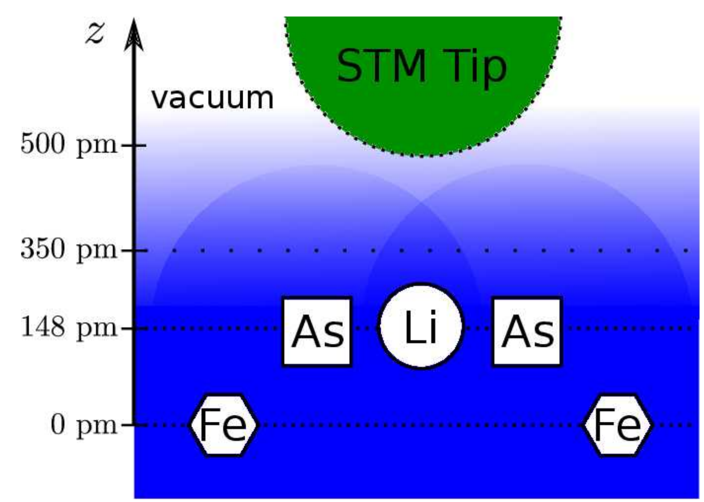
J. Hoffman Rep. Prog. Phys. **74** 124513 (2011)



Tunnelling current:

$$I(V, x, y, z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x, y, z, \epsilon)d\epsilon$$

Local Density Of States (LDOS)
of sample at given energy at the tip position



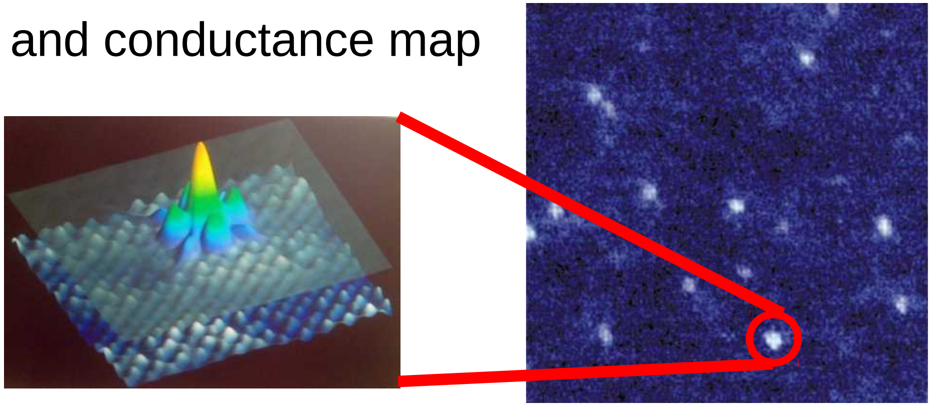
J. Tersoff and D. R. Hamann, PRB **31**, 805 (1985)

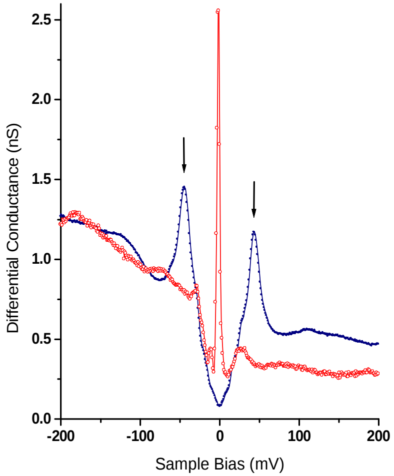
STM: examples

- Cuprates: Zn impurity in BSCCO

Pan et al., Nature **403**, 746 (2000)

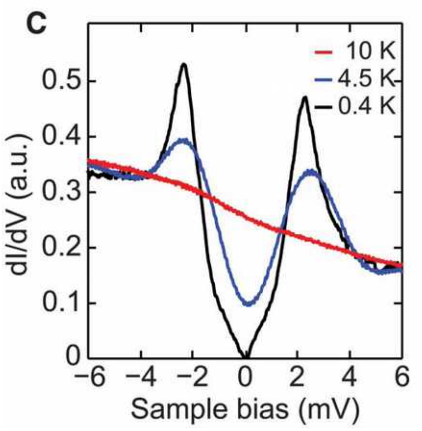
spectra and conductance map



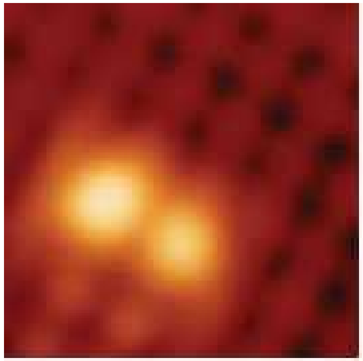


- Fe-SC

FeSe: topograph of Fe centered impurity

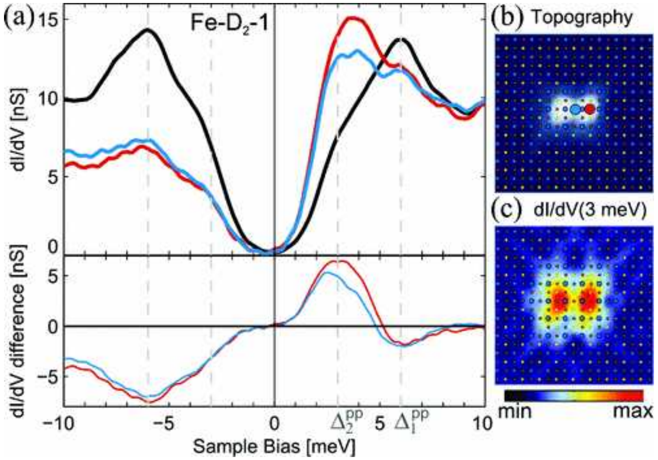


Song et al., Science **332**, 1410 (2011)



Can-Li Song, et al. PRL **109**, 137004 (2012)

LiFeAs: Fe centered impurity



S. Grothe, et al., PRB **86**, 174503 (2012)

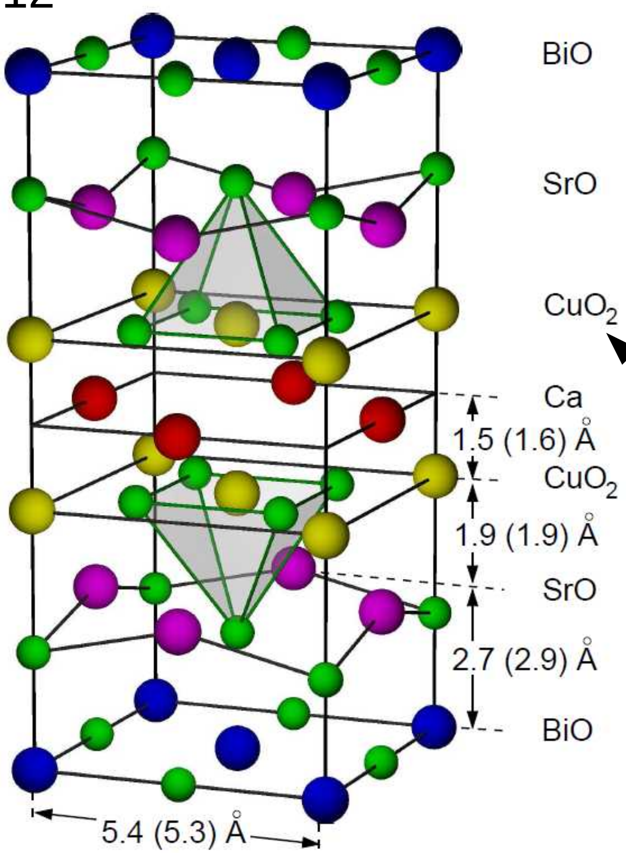
Layered superconductors

- 2 examples: surface atoms ≠ superconducting layer

Cuprates

Bi-2212

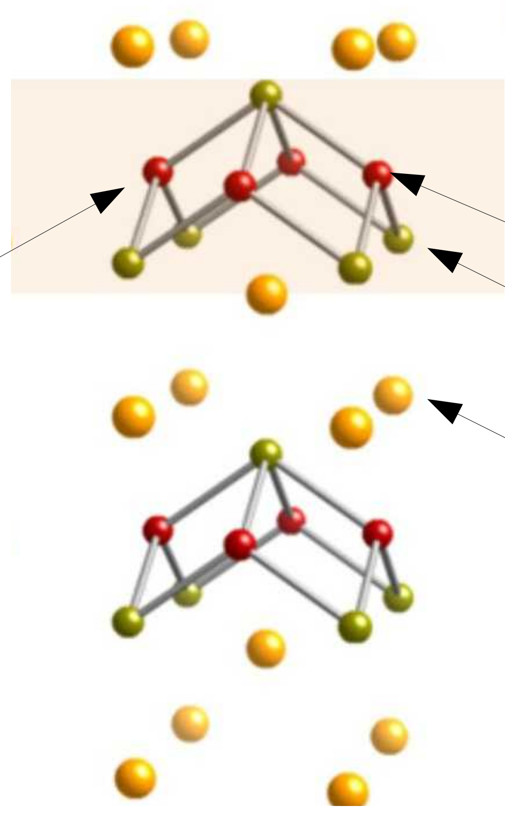
surface: BiO



states at the
Fermi level
Cu-plane
Fe-plane

Iron based superconductors

surface: Li, As?



LiFeAs

“111”

Fe

As

Li

Theoretical approaches: Cuprates

- LDOS: impurity in d-wave superconductor
  - local LDOS: 4 fold pattern
  - low energy bound state

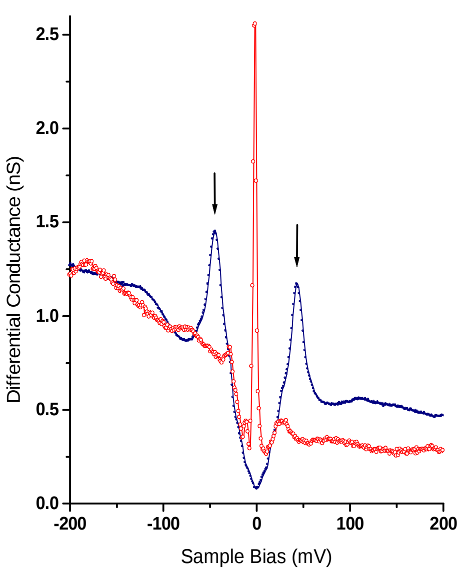
$$\Omega \equiv \Omega' + i\Omega'' = \Delta_0 \frac{\pi c/2}{\ln(8/\pi c)} \left[1 + \frac{i\pi}{2} \frac{1}{\ln(8/\pi c)} \right]$$

J. M. Byers, M. E. Flatté, and D. J. Scalapino Phys. Rev. Lett. **71**, 3363 (1993)

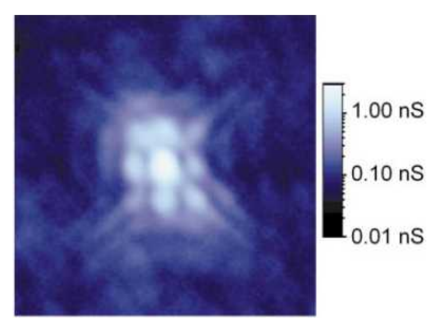
A. V. Balatsky, M. I. Salkola, and A. Rosengren Phys. Rev. B **51**, 15547 (1995)

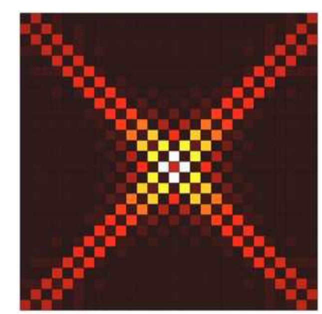
Stamp, Journal of Magnetism and Magnetic Materials, **63**, 429 - 431 (1987) (p-wave)

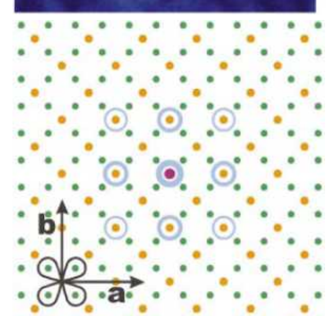
- Comparison to experiment



Pan et al., Nature **403**, 746 (2000)







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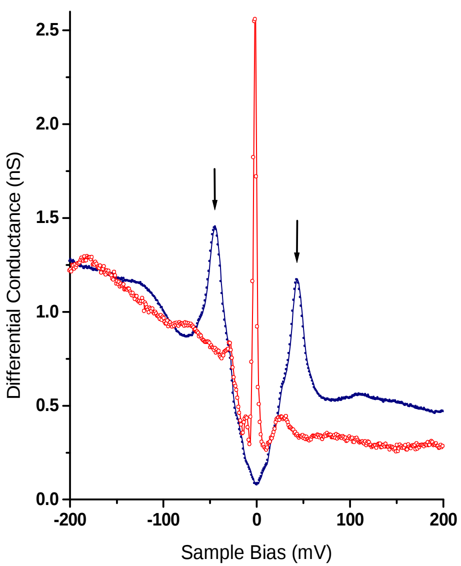
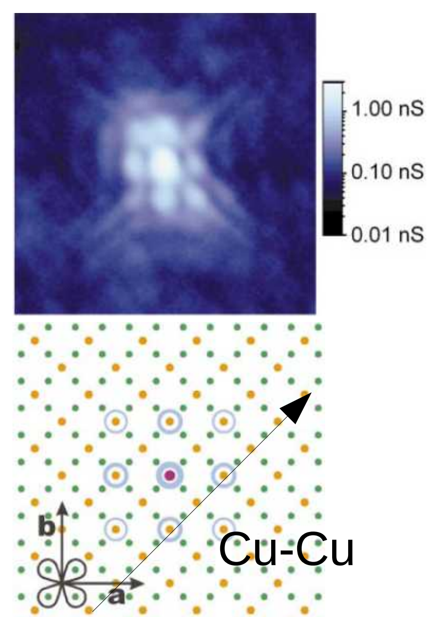
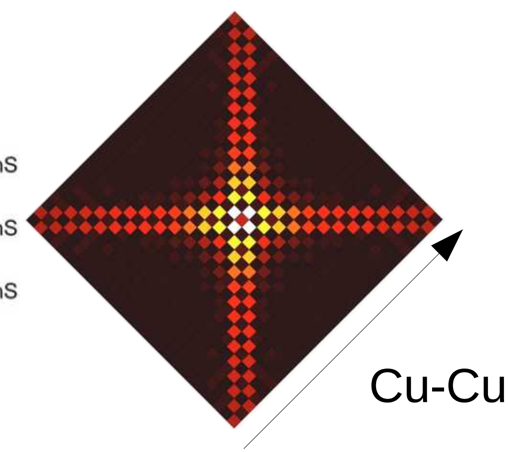


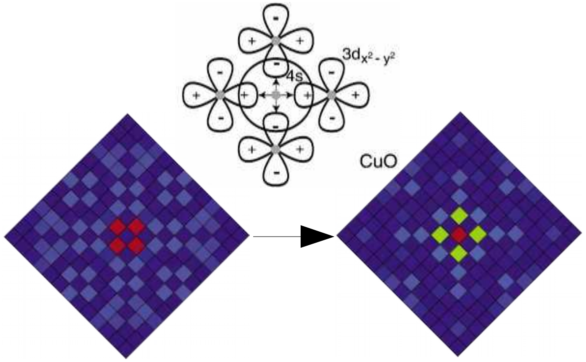
Pan et al., Nature **403**, 746 (2000)





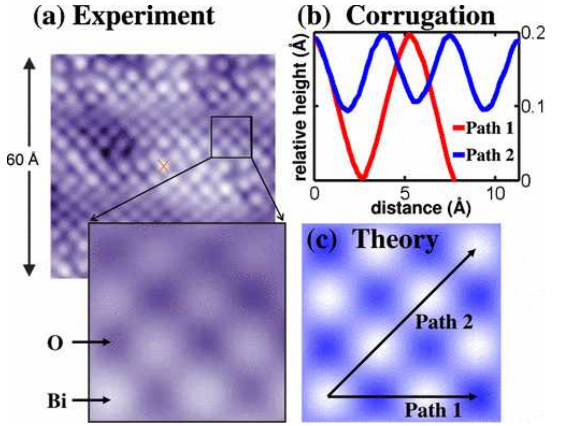
Theoretical approaches: Cuprates

- extended impurity potentials (magnetic Ni impurity) Jian-Ming Tang and Michael E. Flatté PRB **66**, 060504(R) (2002)
- Correlations: "Kondo screening" (magnetic impurity) Anatoli Polkovnikov PRB **65**, 064503 (2002)
- "Filter function": STM tip probes states in the superconducting layer by tunneling matrix elements Martin *et al.*, PRL **88**, 097003 (2002)



- Large tight binding basis set of orbitals + Greens function method to calculate tunneling matrix elements

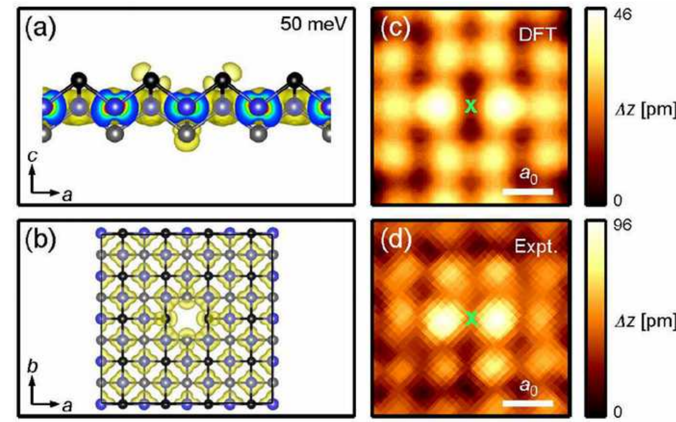
J. Nieminen, *et al.,* PRB **80**, 134509 (2009)



Theoretical approaches: Fe-SC

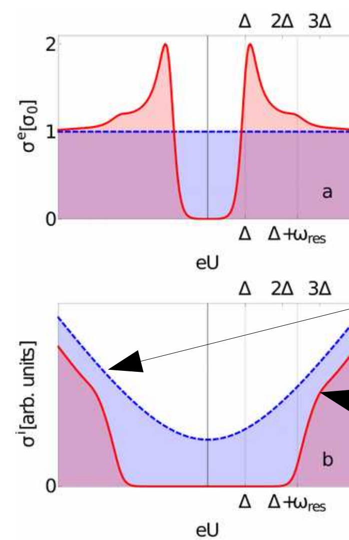
- Identification of nature of impurities in FeSe monolayer (non-SC) by ab-initio calculations

  Dennis Huang et al., Nano Lett., **16** (7), 4224 (2016)



- Inelastic tunneling
  - coupling to bosonic mode
  - signatures of spin fluctuations (real space)

  S. Chi, (…) AK, et al., arXiv:1703.07002



J. R. Kirtley and D. J. Scalapino, PRL **65**, 798 (1990); J. R. Kirtley, PRB **47**, 11379 (1993)
Patrik Hlobil, et al., arXiv:1603.05288 (2016)

normal state

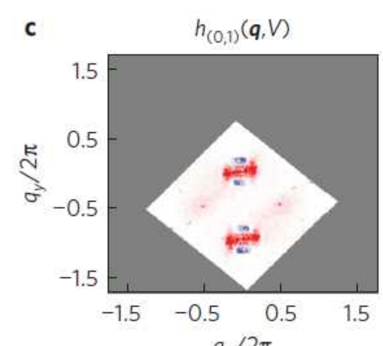
superconducting state

- Wannier method (this talk)

See also: “holographic maps”
Dalla Torre, He, Demler
Nat. Phys., **12**, 1052 (2016)

$$h_G(q,V) = g(q,V)g^*(q+G,V)$$

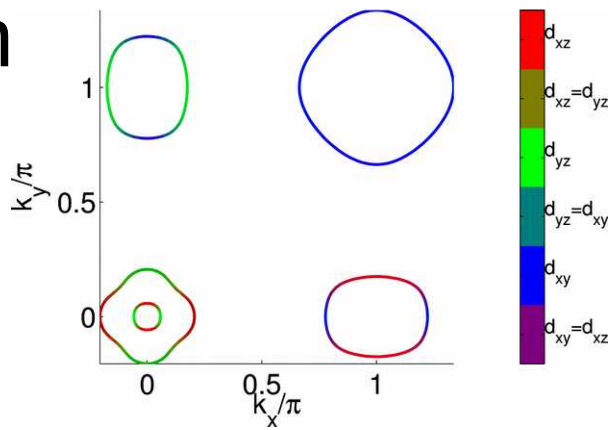
unravel intra-unitcell information

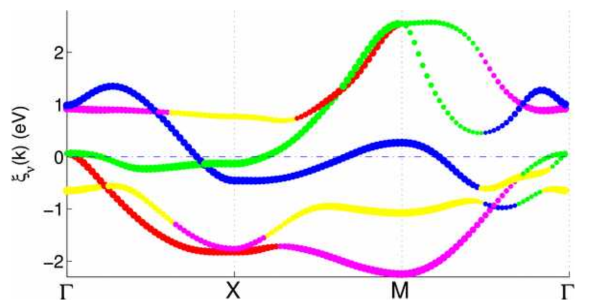


Wannier method: example LiFeAs

- Ab-initio calculation
  - band structure

    5 band model

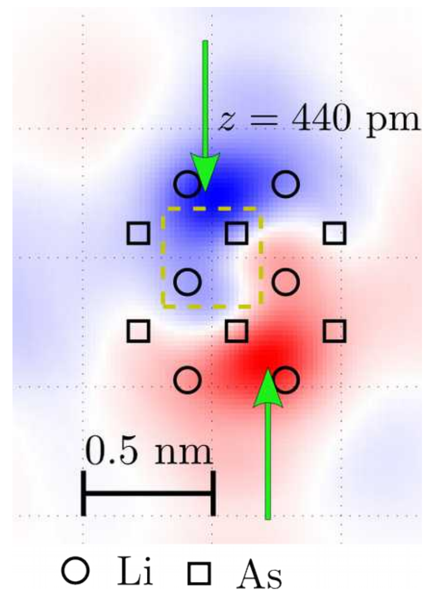


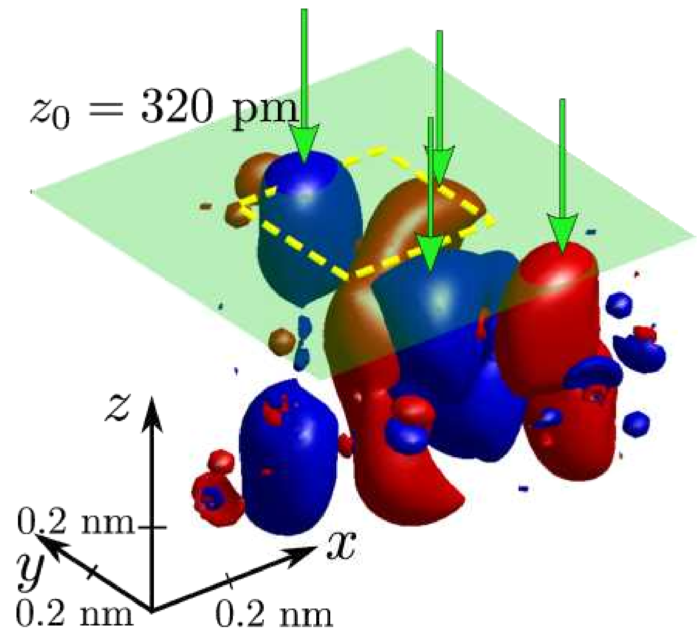


$$H_0 = \sum_{\mathrm{R\,R}',\sigma} t_{\mathrm{R\,R}'} c^\dagger_{\mathrm{R}\,\sigma} c_{\mathrm{R}'\sigma}$$

$$- \mu_0 \sum_{\mathrm{R}\,,\sigma} c^\dagger_{\mathrm{R}\,\sigma} c_{\mathrm{R}\,\sigma}$$

  - Wannier functions (including glide plane symmetry)





Superconductivity

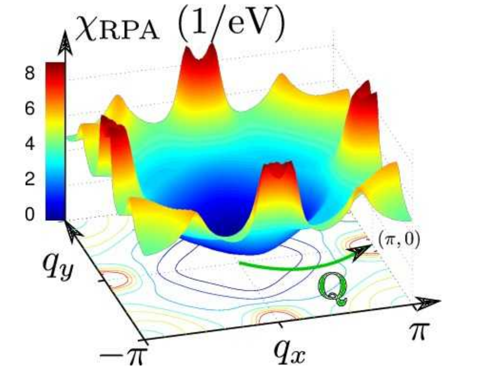
- superconducting order parameter from spin- fluctuation theory

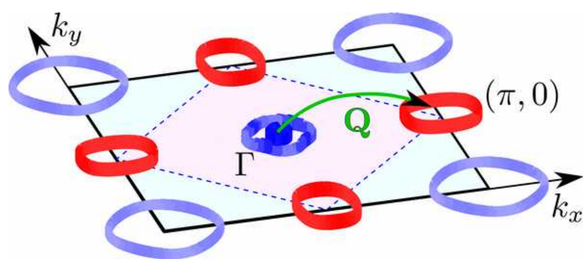
$$H_{\mathrm{BCS}} = -\sum_{\mathrm{R},\mathrm{R}'} \Delta_{\mathrm{R}\,\mathrm{R}'} c^{\dagger}_{\mathrm{R}\uparrow} c^{\dagger}_{\mathrm{R}'\downarrow} + H.c.,$$

- calculate Greens function in superconducting state

$$H_{Nambu} = \begin{pmatrix} H_k & \Delta_k \\ \Delta_k^{\dagger} & -H_{-k} \end{pmatrix}$$

$$G_0(\mathbf{k},\omega) = [\omega - H_{Nambu} + i0^{+}]^{-1}$$





Real space Greens function by Fourier transform

Impurity → engineered

- ab-initio calculation of impurity potential for Co, Ni, Mn in LiFeAs (engineered impurity)

$$H_{\text{imp}} = \sum_{\sigma} V_{\text{imp}} c^{\dagger}_{\mathsf{R}*\sigma} c_{\mathsf{R}*\sigma}$$

$$H = H_0 + H_{\text{BCS}} + H_{\text{imp}}$$

- T-matrix approach to obtain Greens function

  (other methods also possible

  - BdG
  - Gutzwiller mean field

Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey et al., New J. Phys. **19**, 013028 (2017)

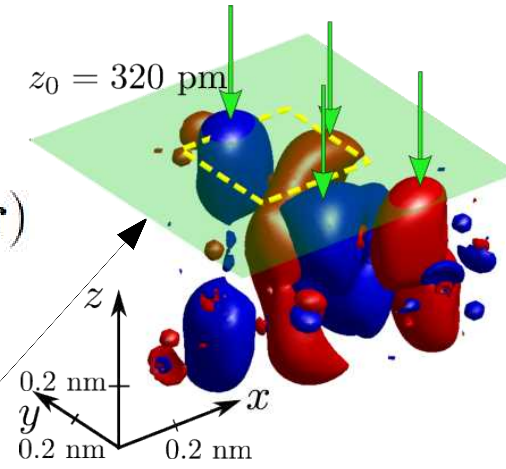
$$\underline{\hat{G}}_{\mathbf{R},\mathbf{R}'}(\omega) = \underline{\hat{G}}^0_{\mathbf{R}-\mathbf{R}'}(\omega) + \underline{\hat{G}}^0_{\mathbf{R}}(\omega)\underline{\hat{T}}(\omega)\underline{\hat{G}}^0_{-\mathbf{R}'}(\omega)$$

$$\underline{\hat{T}}(\omega) = [1 - \underline{\hat{V}}_{\text{imp}}\underline{\hat{G}}(\omega)]^{-1}\underline{\hat{V}}_{\text{imp}}$$

lattice Green function (state of the art)

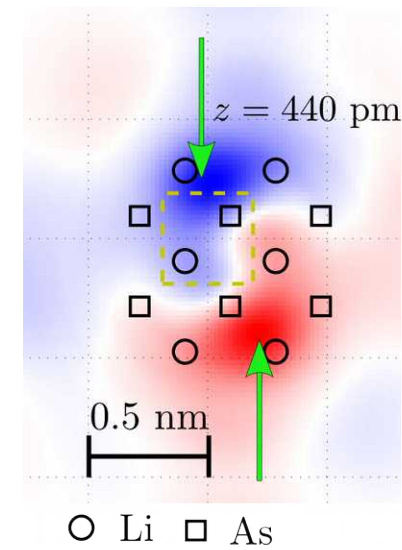
cLDOS

- Basis transformation $\psi_\sigma(\mathbf{r}) = \sum_{\mathbf{R}\mu} c_{\mathbf{R}\mu\sigma} w_{\mathbf{R}\mu}(\mathbf{r})$



$$\underline{\hat{G}}_{\mathbf{R},\mathbf{R}'}(\omega) = \underline{\hat{G}}^0_{\mathbf{R}-\mathbf{R}'}(\omega) + \underline{\hat{G}}^0_{\mathbf{R}}(\omega)\underline{\hat{T}}(\omega)\underline{\hat{G}}^0_{-\mathbf{R}'}(\omega)$$

surface Wannier function with phases



$$\underline{G}(\mathbf{r},\mathbf{r}';\omega) = \sum_{\mathbf{R},\mathbf{R}',\mu\nu} \underline{\hat{G}}^{\mu,\nu}_{\mathbf{R},\mathbf{R}'}(\omega) w_{\mathbf{R}\mu}(\mathbf{r}) w_{\mathbf{R}'\nu}(\mathbf{r}')$$

continuum position

nonlocal contributions

lattice Green function

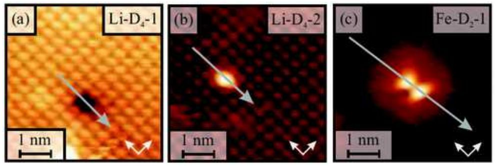
continuum Local Density Of States (cLDOS) of sample at given energy at the tip position

$$\rho(\mathbf{r},\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,G(\mathbf{r},\mathbf{r};\omega)$$

LiFeAs: Questions

- Properties of the order parameter (sign-change)
- Interpretation of
  - impurity shapes

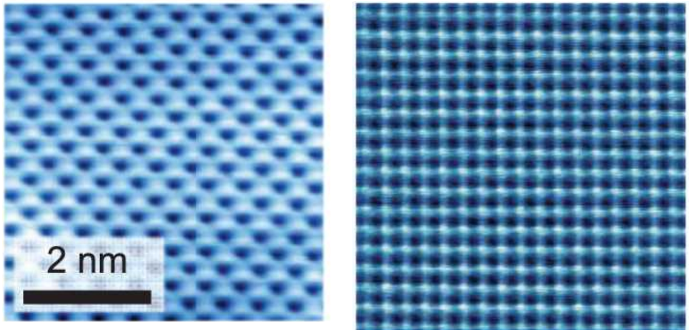
R. Schlegel, et al., Phys. Status Solidi B, **254**: 1600159 (2017)



Hanaguri, unpublished (KITP 2011)

“Dot” “Trench” “Dumbbell”

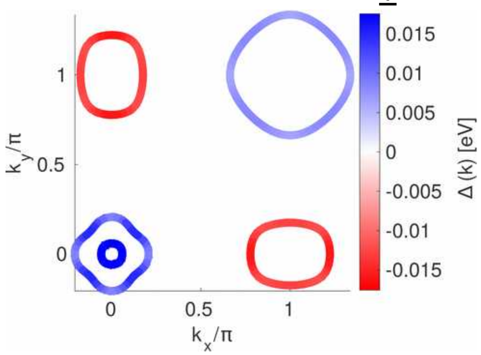
  - registered “surface lattice” in STM



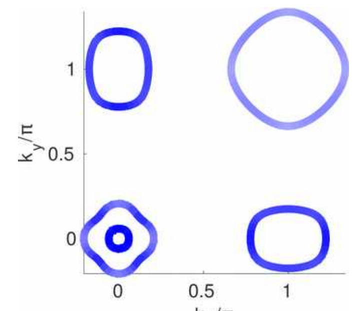
LiFeAs: Li or As lattice?

Shun Chi, et al., PRL 109, 087002 (2012)
T. Hanaguri, et al. PRB 85, 214505 (2012)
S. Grothe, et al., PRB 86, 174503 (2012)
J. -X. Yin, et al., arXiv, 1602.04949 (2016)

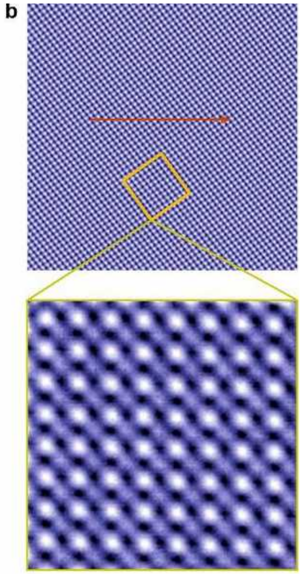
conventional $s_{\pm}$



conventional s_{++}

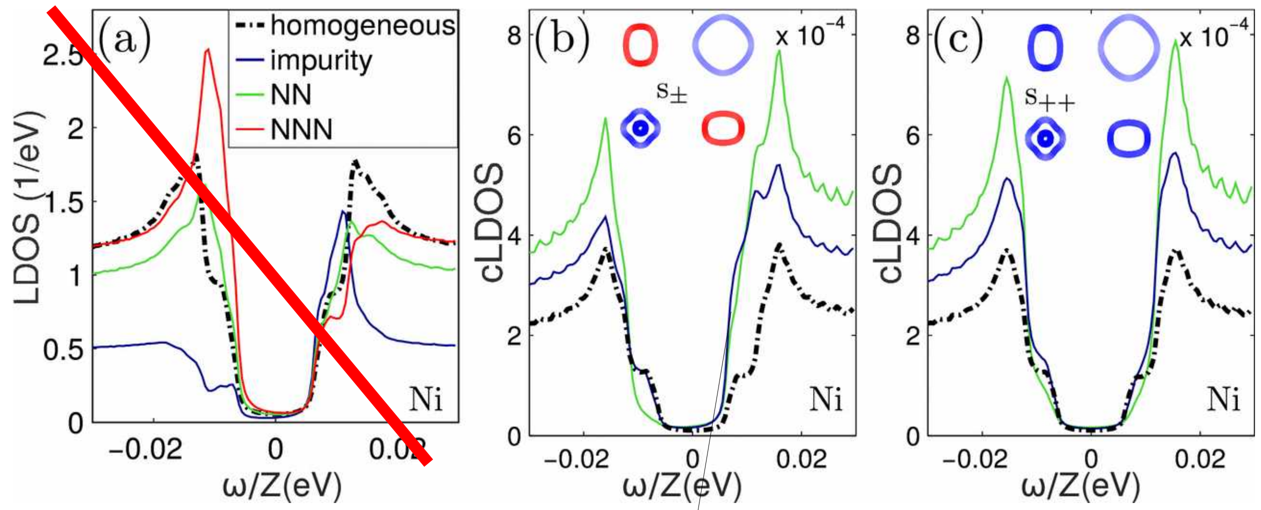


Y. Wang, A. Kreisel, et al.
Phys. Rev. B **88**, 174516 (2013)
Z. P. Yin, K. Haule, G. Kotliar
Nature Physics **10**, 845-850 (2014)
T. Saito, et al.
Phys. Rev. B **90**, 035104 (2014)
F. Ahn, et al. Phys. Rev. B **89**, 144513 (2014)



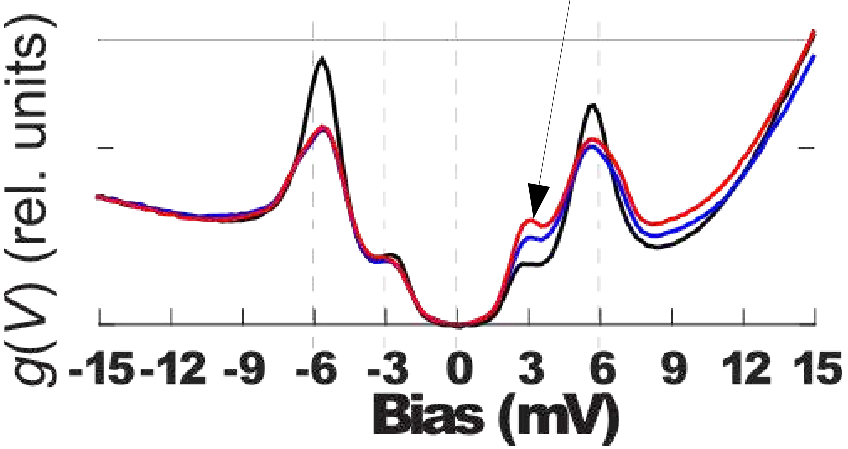
LiFeAs: spectra

- evidence for sign-changing order parameter by in-gap state with engineered impurity



lattice LDOS: strong response at negative bias

$$0 \approx 1 - V_{\text{imp}}^{\mu\mu} G^0_{\mathbf{R}=0}(\omega)^{\mu\mu}$$

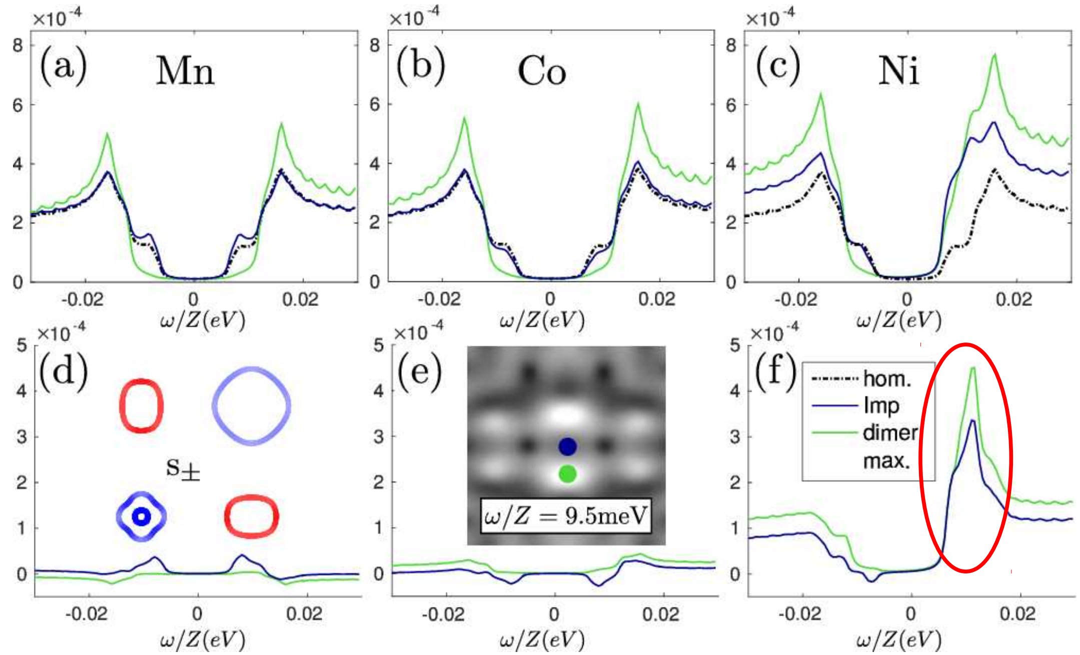


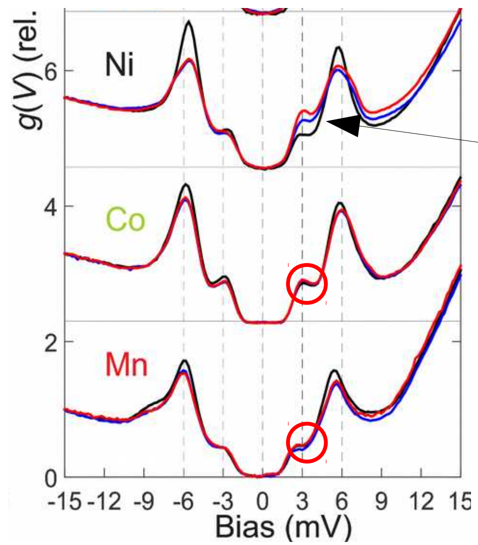
S. Chi, (...) , **A. Kreisel**, *et al.*
Phys. Rev. B **94**, 134515 (2016)

LiFeAs: spectra

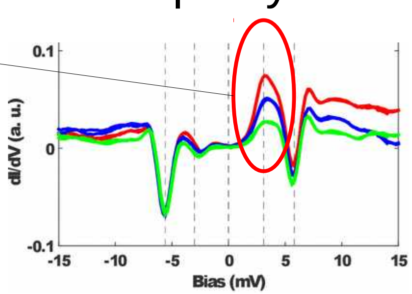
- sequence of impurity potentials from ab-initio calculation correct, but overall renormalization downwards required [correlation effects]

Peter O. Sprau, …, A. Kreisel, et al.
arXiv:1611.02134
A. Kreisel, et al.
arXiv:1611.02643





relative spectra
Ni impurity

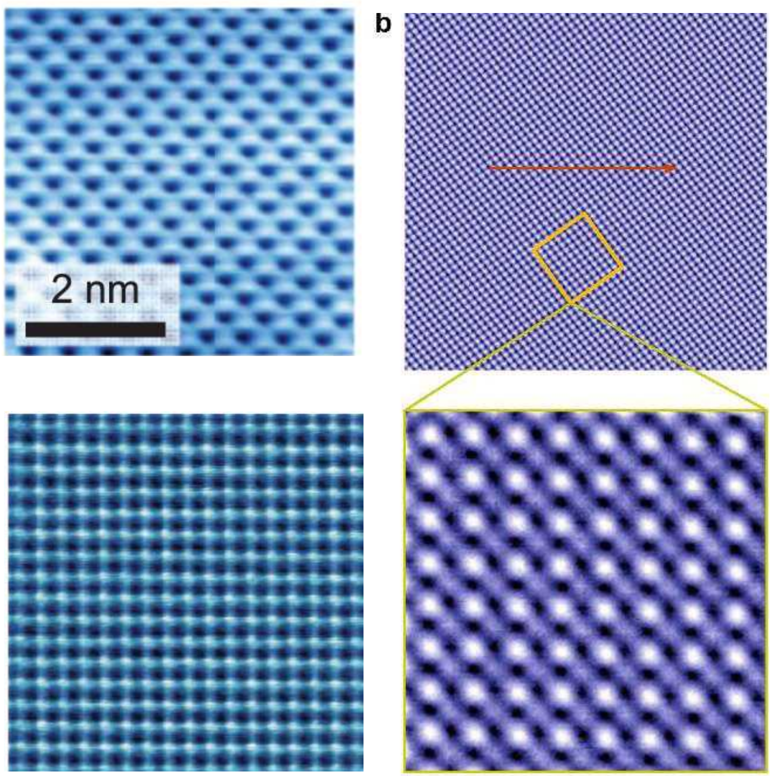


S. Chi, (...) , **A. Kreisel**, *et al.*
Phys. Rev. B **94**, 134515 (2016)

Height and current dependence of topographs

- experiment: Li or As lattice?

height maxima at Li positions!?
counter-intuitive from chemistry point of view



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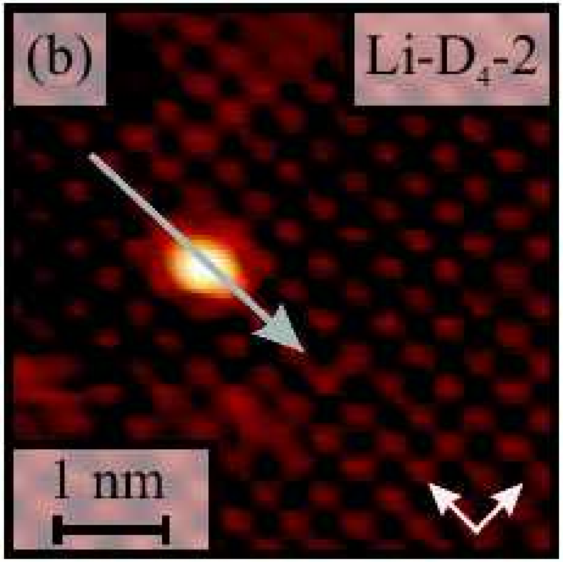
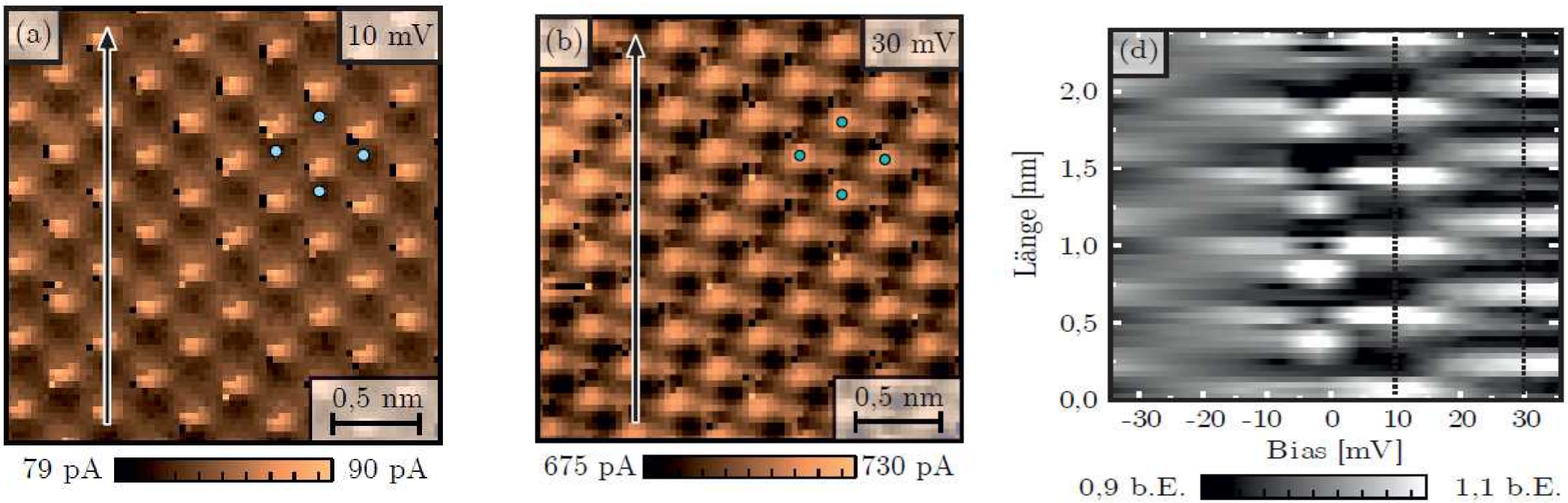
J. -X. Yin, et al., arXiv, 1602.04949 (2016)



R. Schlegel, et al., Phys. Status Solidi B, **254**: 1600159 (2017)

Further experimental evidences?

experiment (current maps)



Ronny Schlegel, Dissertation, TU Dresden
(thanks to C. Hess)

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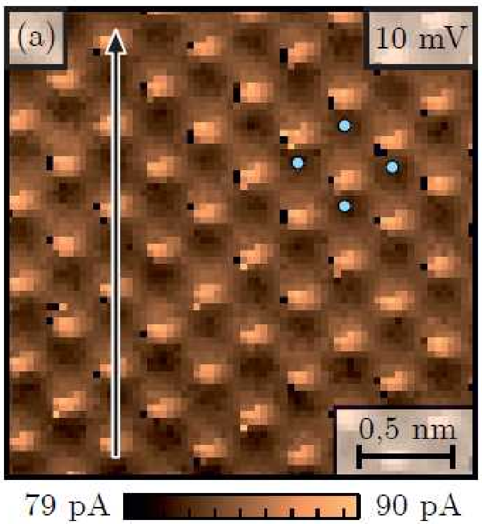
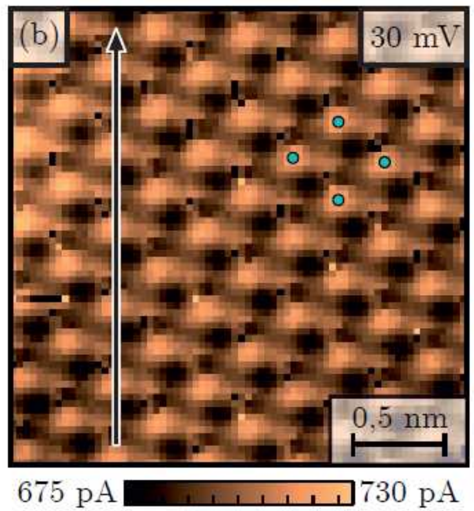
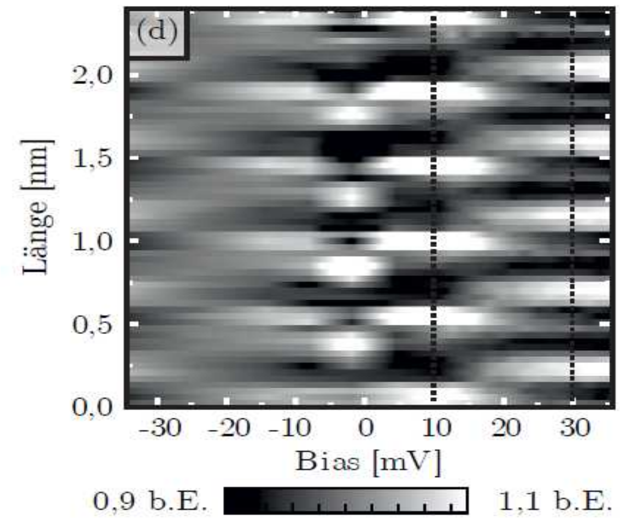
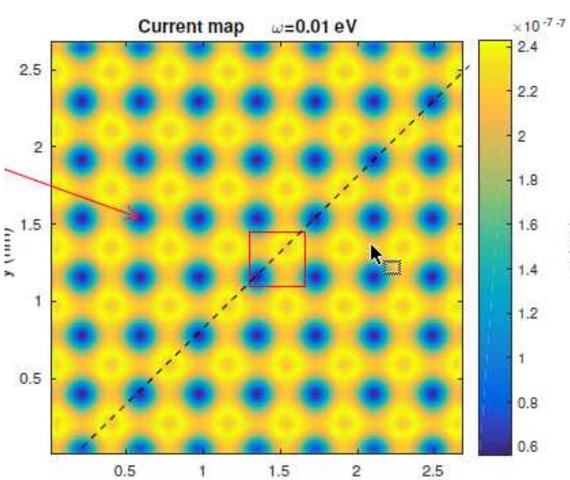


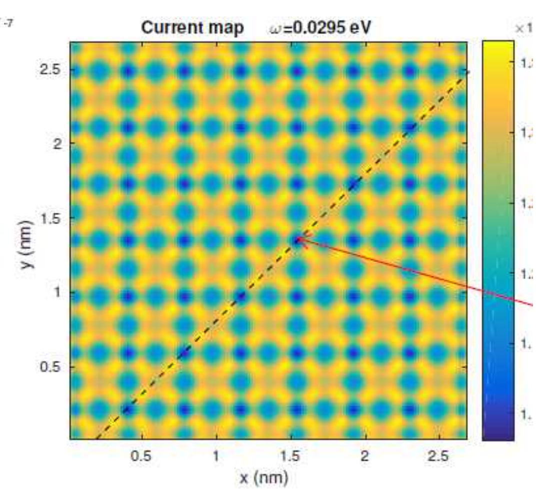


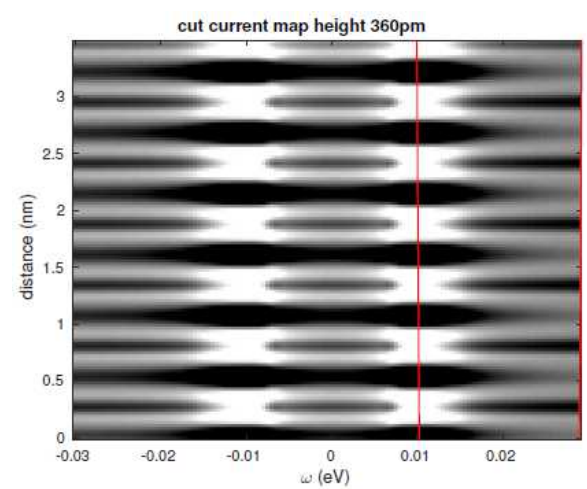


Ronny Schlegel, Dissertation, TU Dresden
(thanks to C. Hess)

theory





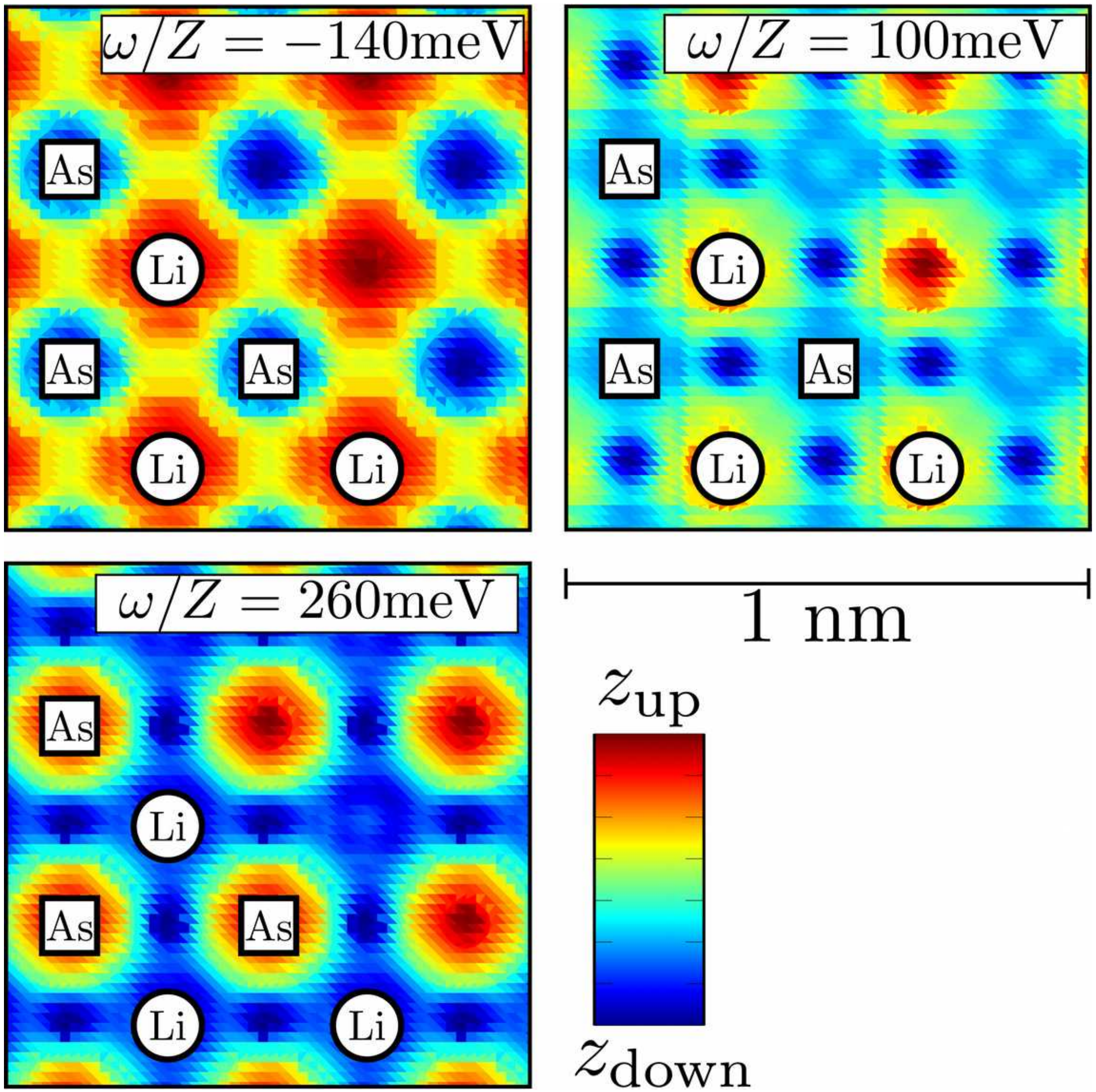


Simulation of topographs

- solve for $z(x, y)$

$$I_0 = \frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} d\omega \; \rho(x, y, z(x, y), \omega)$$

- switching of height maxima as a function of bias voltage

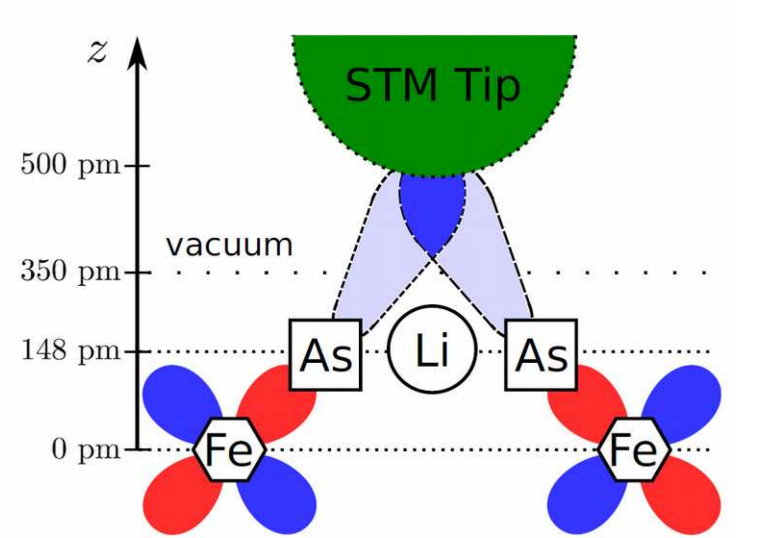


Results
registered surface lattice in STM

- tunneling into states described by Wannier functions

$$G(\mathrm{r},\mathrm{r}';\omega)=\sum_{\mu,\nu,\mathrm{R},\mathrm{R}'} G(\mathrm{R},\mu,\mathrm{R}',\nu;\omega)\,w_{\mathrm{R},\mu}(\mathrm{r})\,w^{*}_{\mathrm{R}',\nu}(\mathrm{r}')$$

- registered lattice switches as function of bias and current

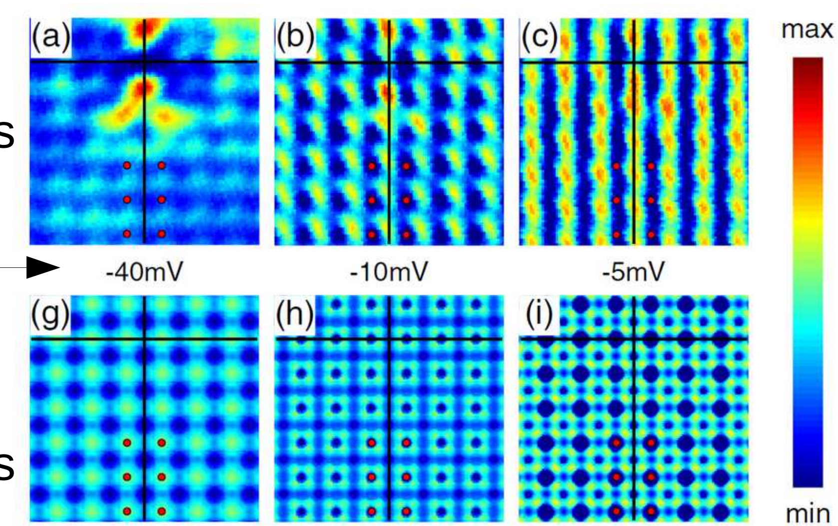


"Li lattice" "As lattice"

measured topographies

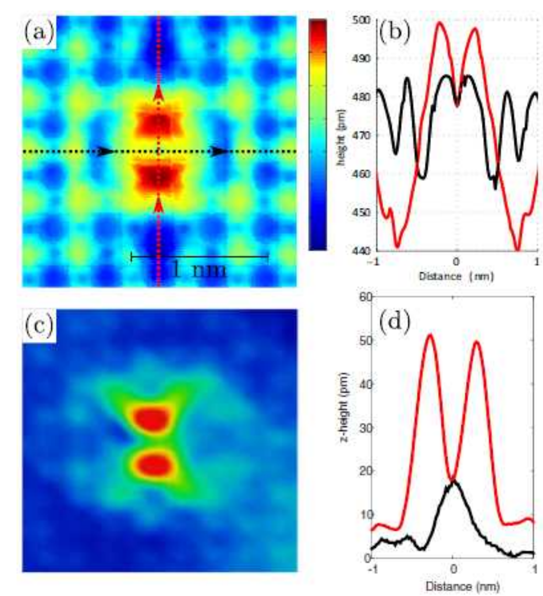
bias

simulated topographies



simulated topography close to strong imp.

measured topography close to Ni



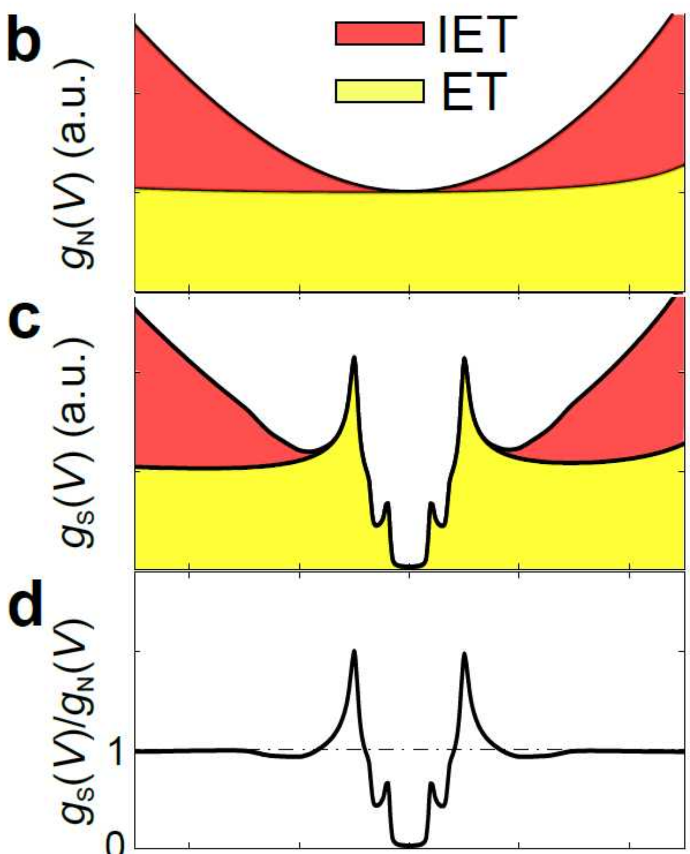
Inelastic tunneling: coupling to spin fluctuations

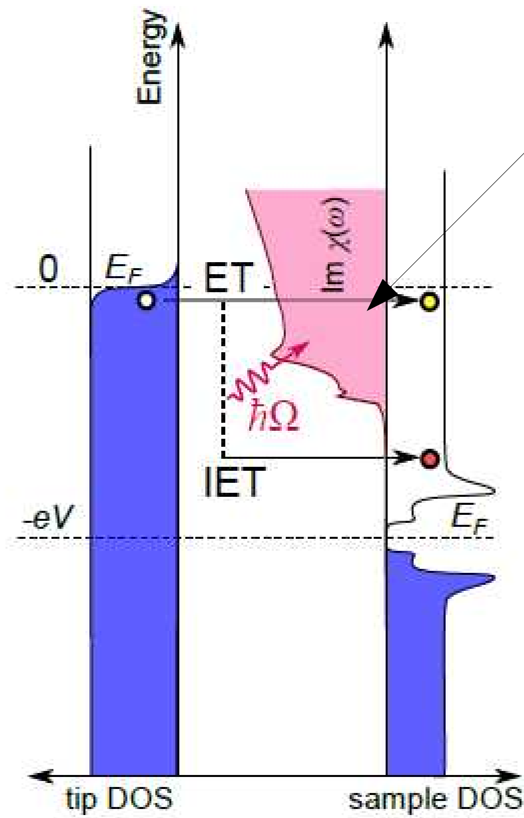
- Inelastic contribution

$$g_{\mathrm{inel}}(V) \propto \int_0^{eV} \chi(\omega)\rho(eV-\omega)\,\mathrm{d}\omega$$

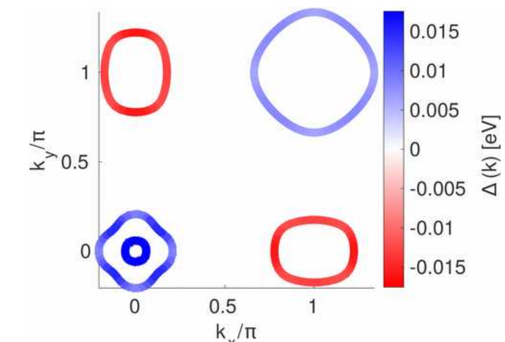
Spin fluctuations: two gap superconductor (LiFeAs), double resonance

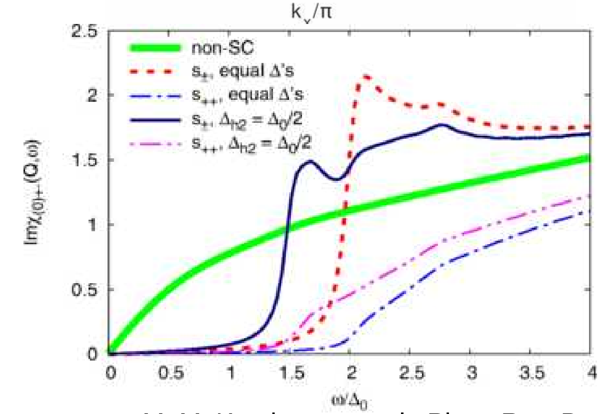
- Dip-hump feature





J. R. Kirtley and D. J. Scalapino, PRL **65**, 798 (1990); J. R. Kirtley, PRB **47**, 11379 (1993)
Patrik Hlobil, et al., arXiv:1603.05288 (2016)





M. M. Korshunov, et al., Phys. Rev. B 94, 094517 (2016)

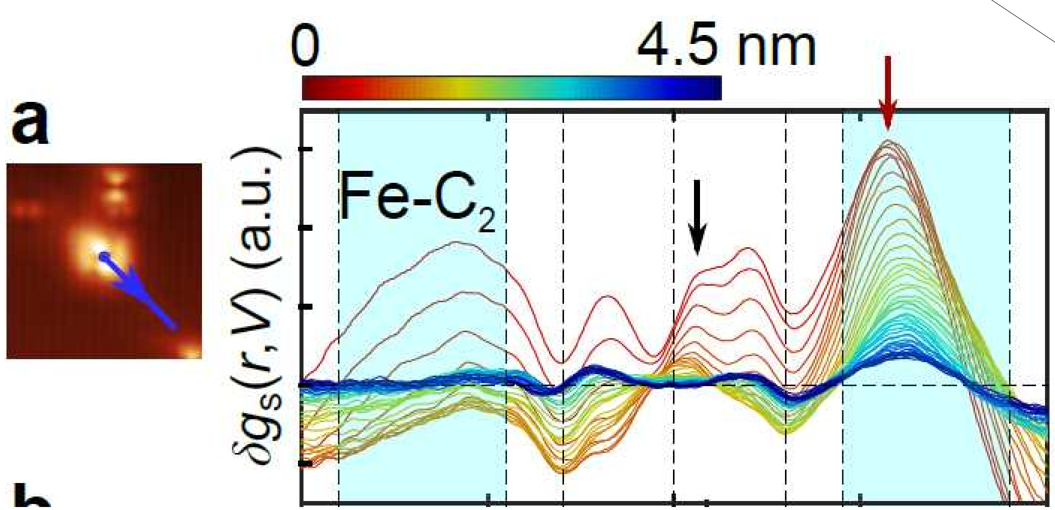
Imaging spin fluctuations in real space

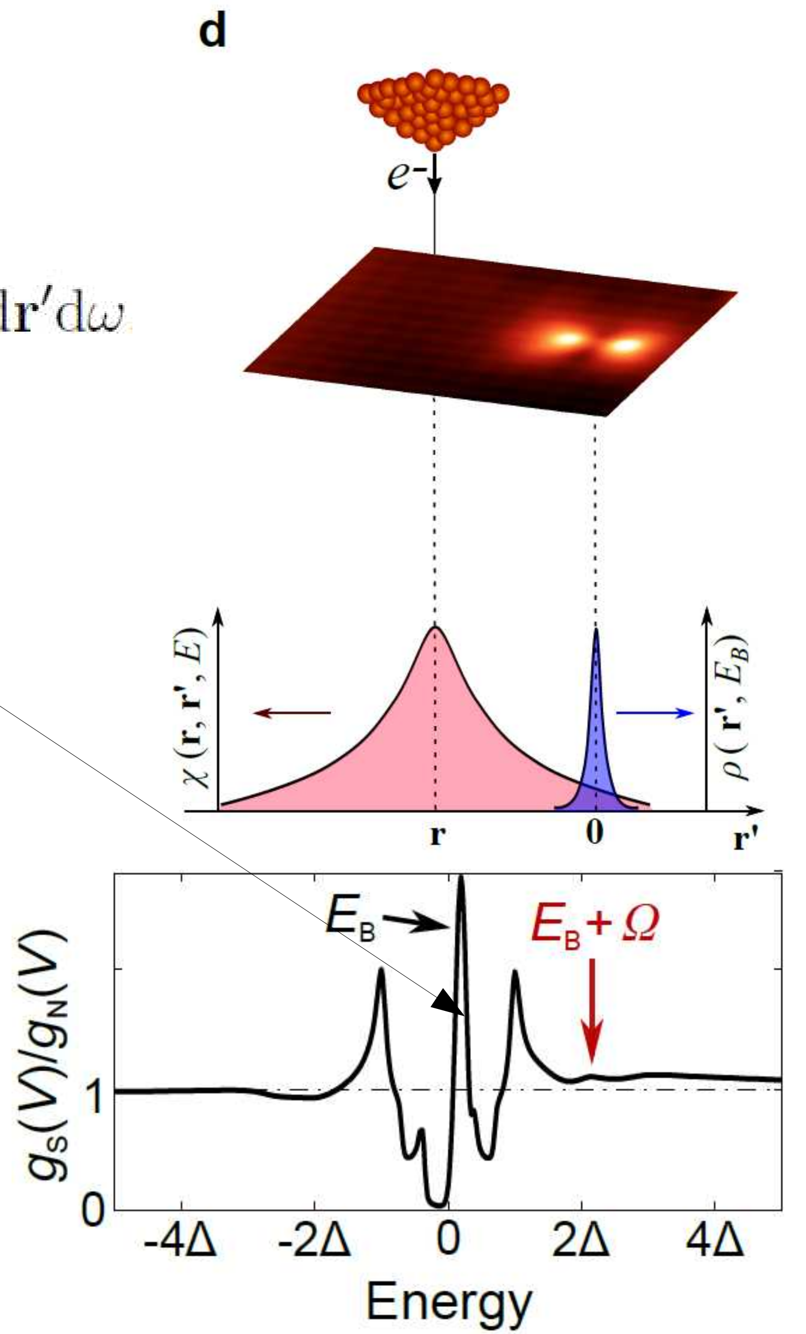
- real space structure

$$g_{\rm inel}(\mathbf{r},V) \propto \int_0^{eV}\int \rho(\mathbf{r}',eV-\omega)\,\chi(\mathbf{r},\mathbf{r}',\omega)\,\mathrm{d}\mathbf{r}'\mathrm{d}\omega$$

S. Chi, (…) AK, et al., arXiv:1703.07002

- in presence of impurity



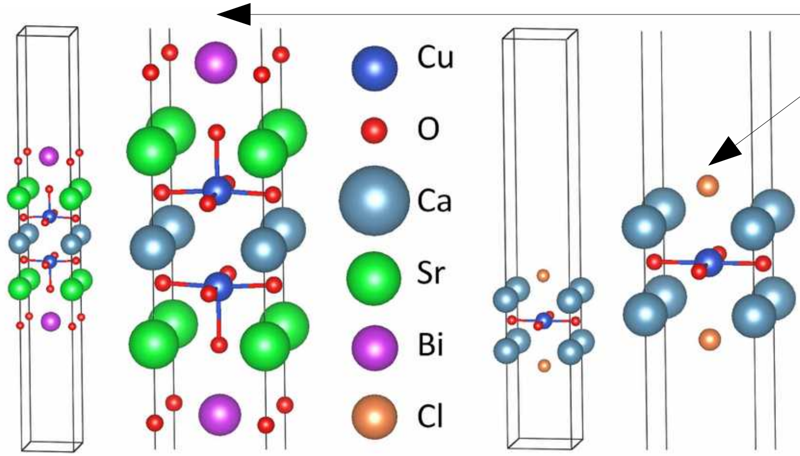


Fast spatial decay of impurity resonance, slow decay of dip-hump → spin fluctuations (real space)

Other systems?

- Cuprates

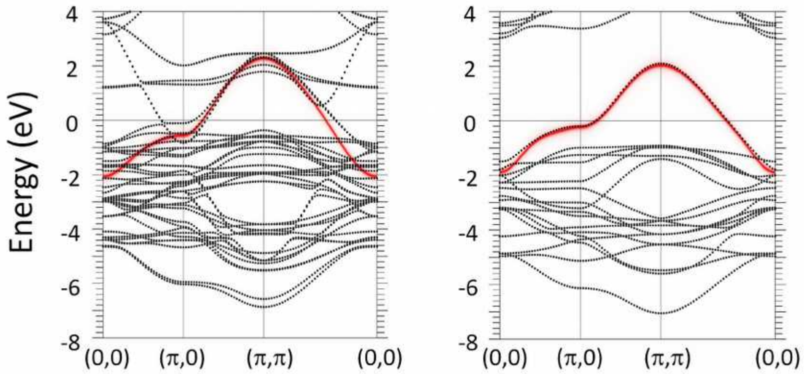
$Bi_2Sr_2CaCu_2O_8$

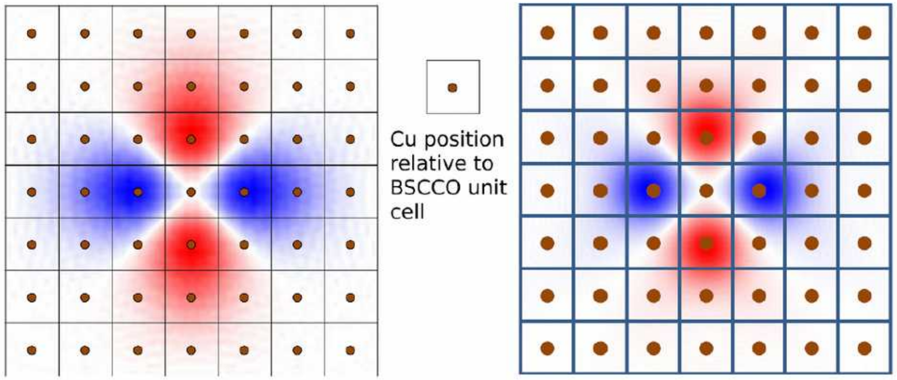


$Ca_2CuO_2Cl_2$

Surface
BiO vs. CaCl
and tunneling path
very different

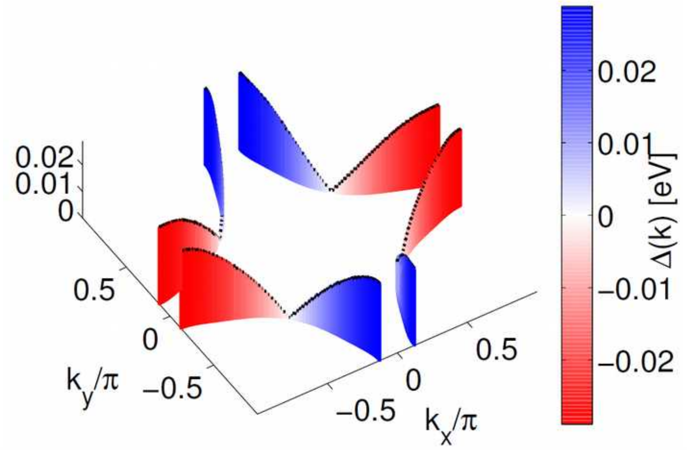
Ab initio calculation:
1 band model
+Wanner function





similar properties
dictated by
crystal symmetry

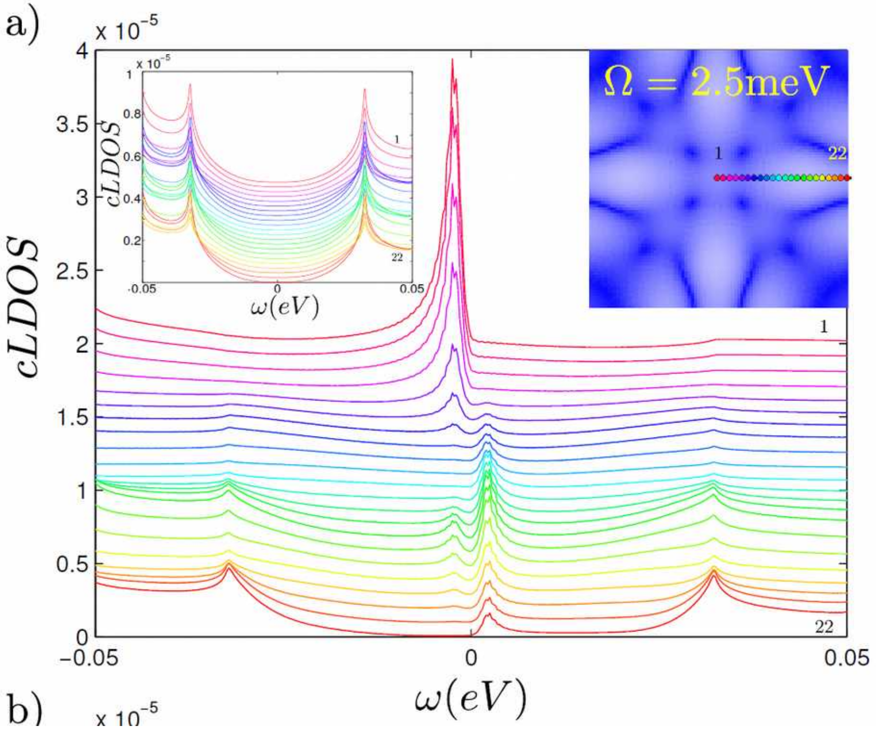
$Bi_2Sr_2CaCu_2O_8 \leftrightarrow Ca_2CuO_2Cl_2$

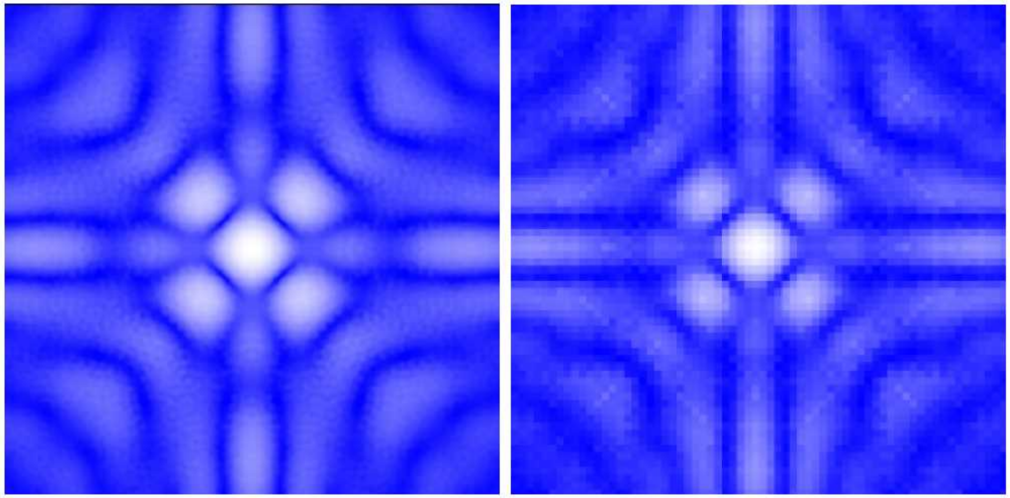


- superconductivity:
  d-wave order parameter
- T-matrix calculation+ Wannier method

$$G(\mathsf{r},\mathsf{r}';\omega)=\sum_{\mu,\nu,\mathsf{R},\mathsf{R}'}G(\mathsf{R},\mu,\mathsf{R}',\nu;\omega)w_{\mathsf{R},\mu}(\mathsf{r})w^*_{\mathsf{R}',\nu}(\mathsf{r}')$$

- strong impurity
  spectra + conductance map



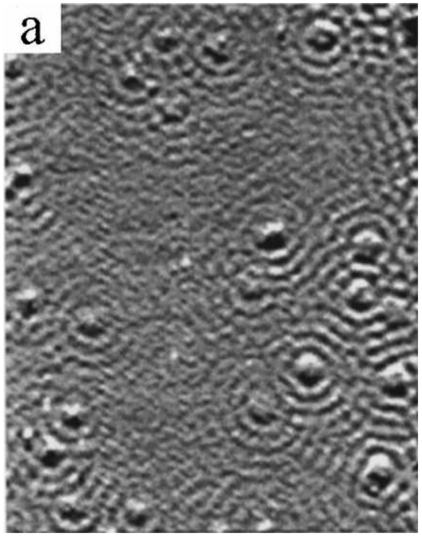


$Bi_2Sr_2CaCu_2O_8$ $Ca_2CuO_2Cl_2$

Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey et al., New J. Phys. **19**, 013028 (2017)
Choubey, et al. (in preparation)

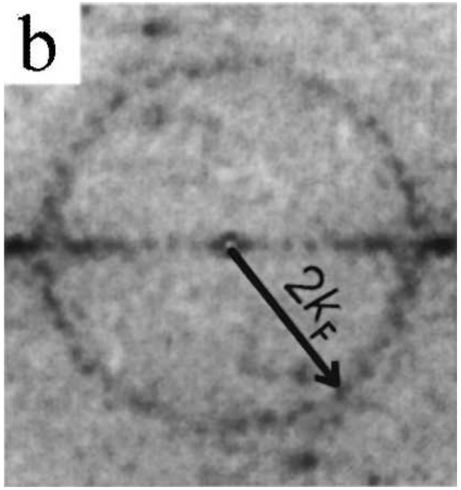
Quasiparticle Interference (QPI)

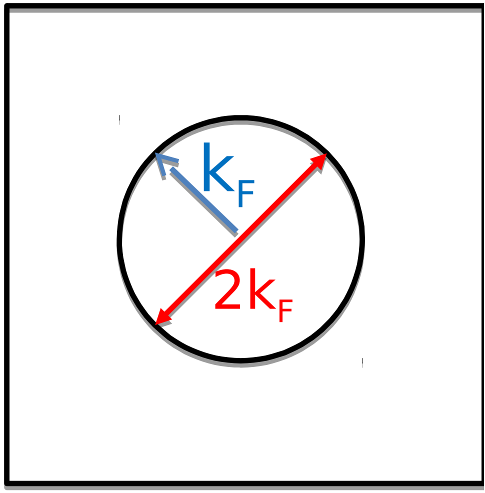
- STM on normal metal (Cu)
  - impurities
  - Friedel oscillations



L. Petersen, et al.
PRB **57**, R6858(R)
(1998)

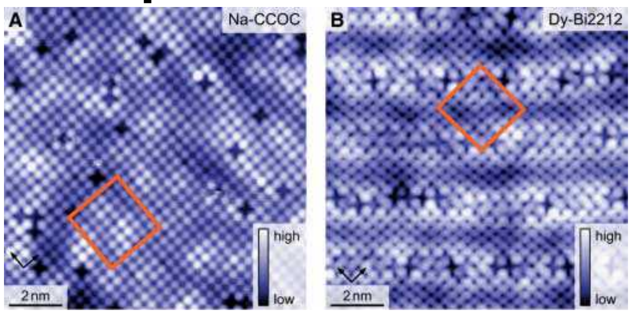
- Fourier transform of conductance map
  - mapping of constant energy contour



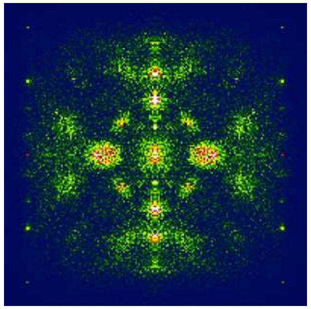


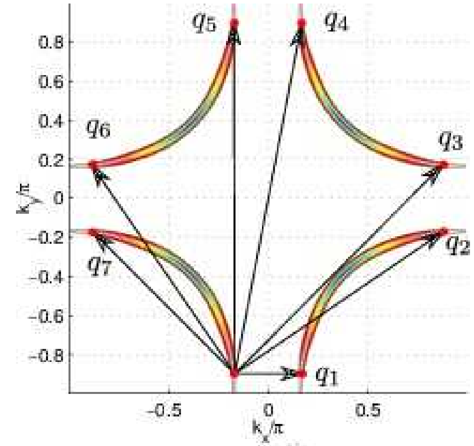
QPI in superconductors

- Fourier transform of differential conductance maps

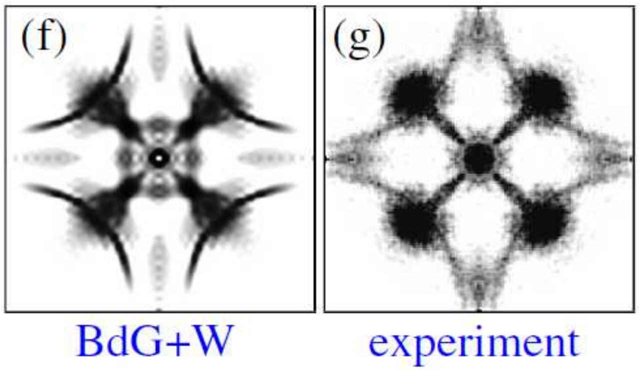


FT



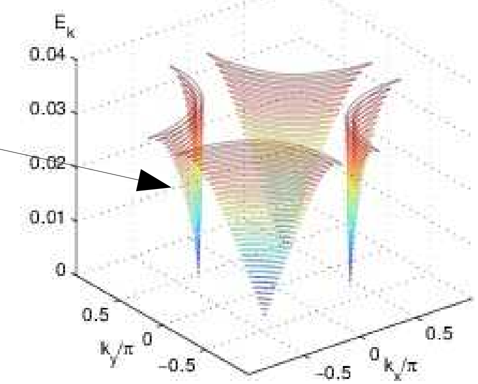


K Fujita et al. Science **344**, 612 (2014)



A. Kreisel, et al., PRL **114**, 217002 (2015)

$$E_{\mathsf{k}} = \pm\sqrt{\epsilon_{\mathsf{k}}^2 + \Delta_{\mathsf{k}}^2}$$



Trace back Fermi surface+measure superconducting gap function

octet model: 7 scattering vectors between regions of high DOS

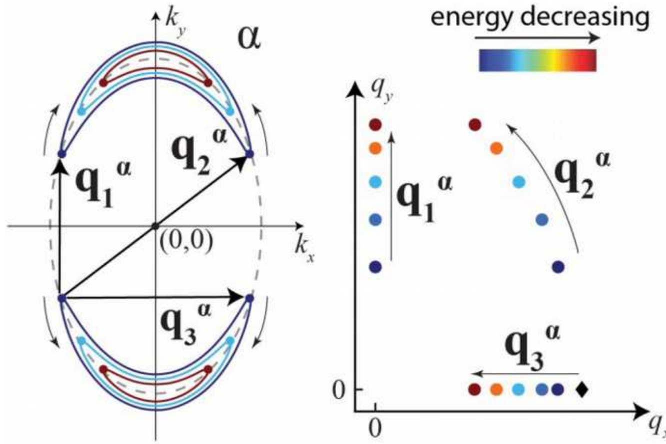
FeSe BQPI

- Peaks follow high density of states of constant energy contours $E_{\mathbf{k}} = \pm\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$

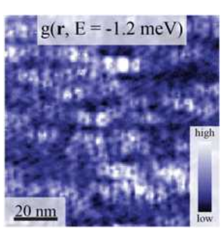
Sprau, et al., arXiv 1611.02134

- Measure gap and Fermi surface

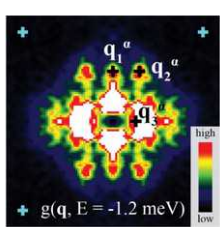
CEC: constant energy contour
Expected scattering vectors



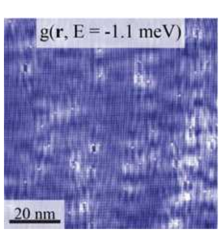
Dispersion of QPI peaks
q(E) → k(E) → E(k)



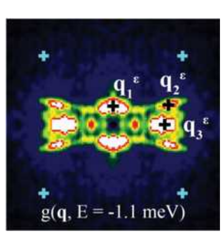
FT



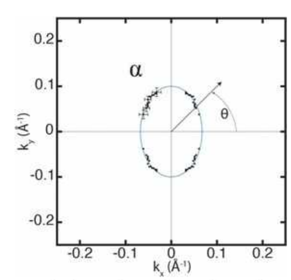
Conductance maps

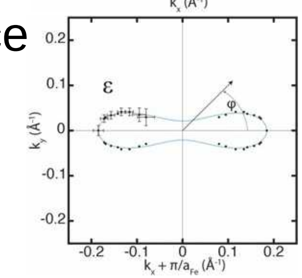


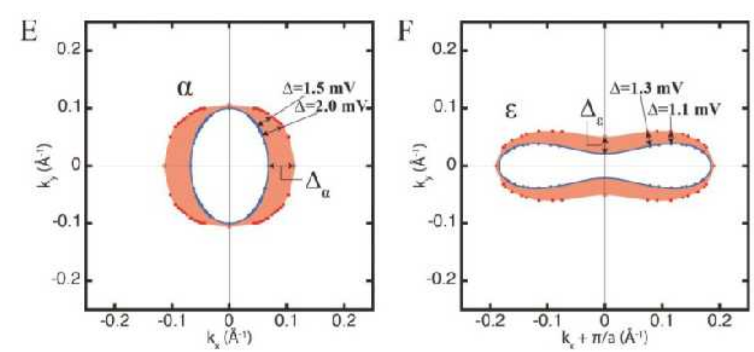
FT



Trace back Fermi surface

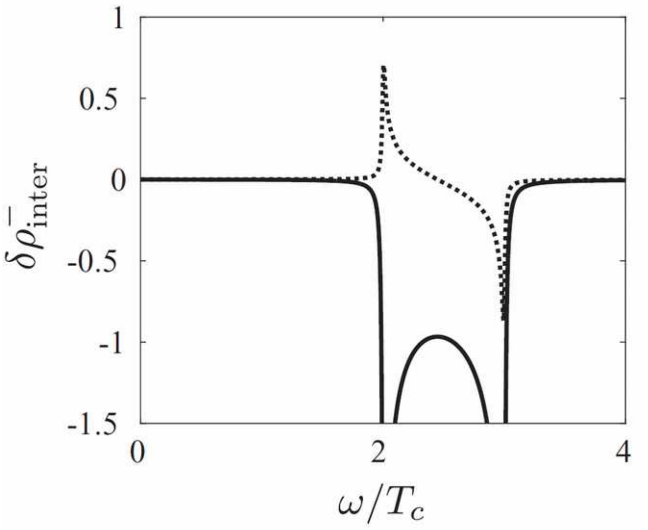






→ gap magnitude, sign?

Phase sensitive measurement



- consider:

$$\rho_-(\vec{q},\omega) = Re\{g(\vec{q},+\omega)\} - Re\{g(\vec{q},-\omega)\}$$

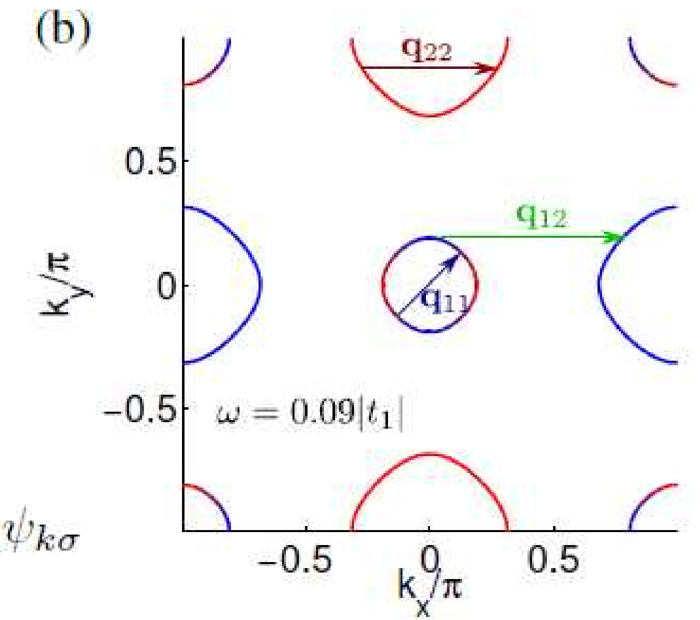
Hirschfeld et al., PRB **92**, 184513 (2015)

- integrate over scattering processes involving sign change
- s++: sign change in signal
- s+-: no sign change in signal
- demonstrated for structureless band structure, single centered impurity, Born limit

More realistic: 2 band model

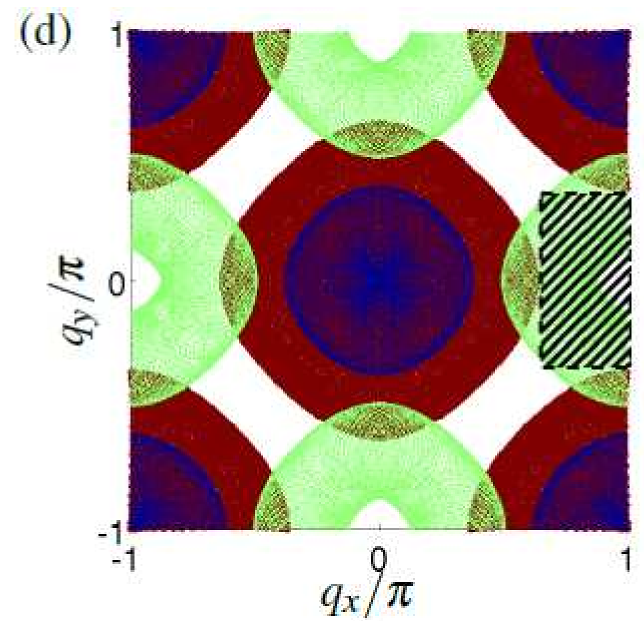
- Fermi surface

$$\mathcal{H}_0 = \sum_{k\sigma} \psi^\dagger_{k\sigma} \left[(\epsilon_+(k) - \mu)\tau_0 + \epsilon_-(k)\tau_3 + \epsilon_{xy}(k)\tau_1 \right] \psi_{k\sigma}$$



- JDOS for obtaining sign changing scattering vectors

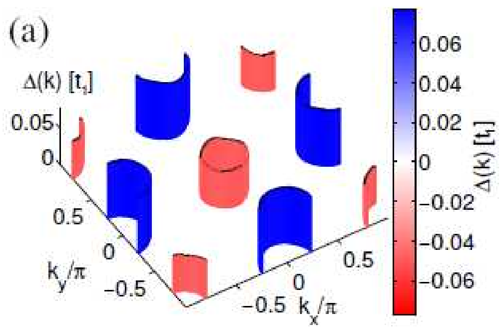
$$\mathcal{H}_{\rm imp} = \sum_{\mu,\sigma=\pm} (V_{\rm imp} - \sigma J) c^\dagger_{i'\mu\sigma} c_{i'\mu\sigma}$$

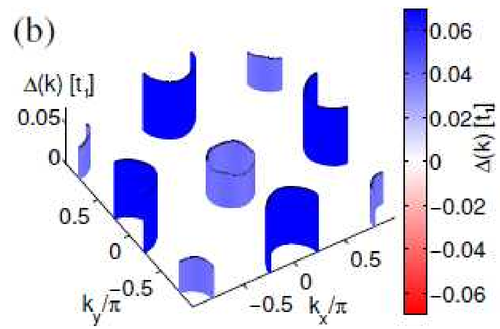


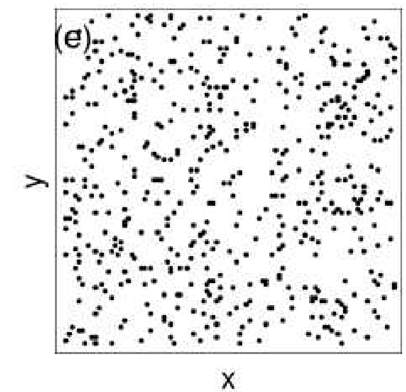
Martiny, et al., arXiv:1703.04891v1

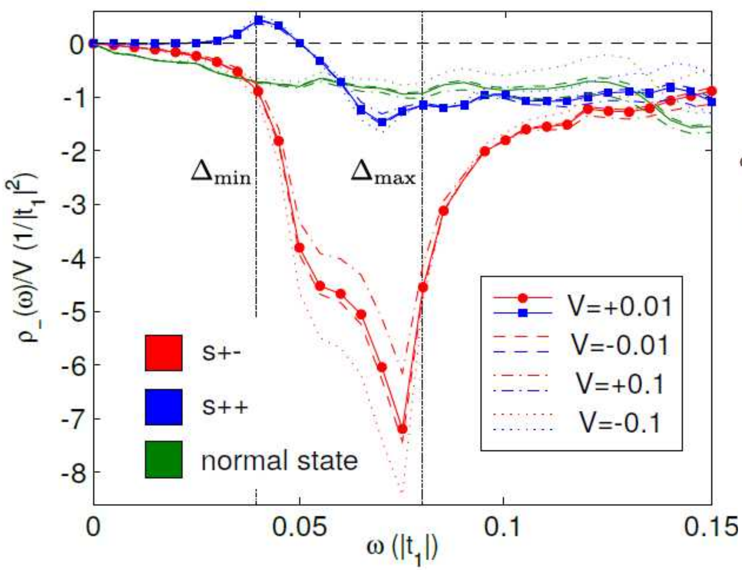
Results: possible ways to recover signal

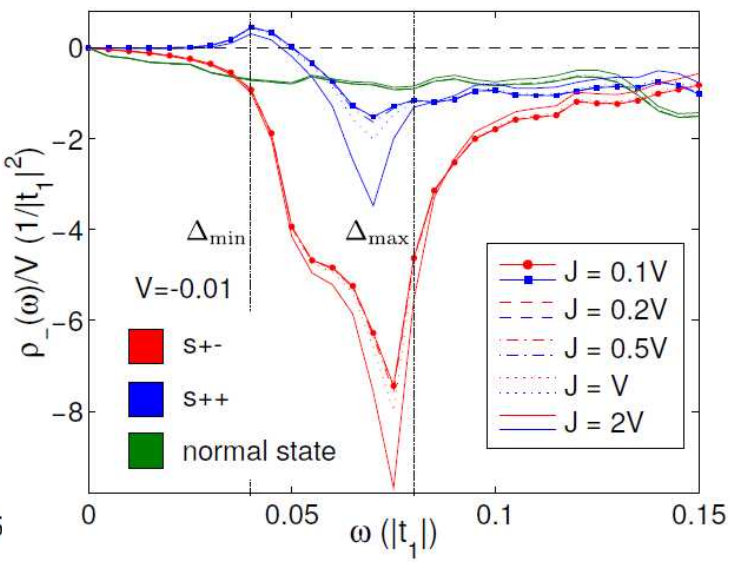
- Calculate antisymmetrized density response $\rho_{-}(\vec{q},\omega) = Re\{g(\vec{q},+\omega)\} - Re\{g(\vec{q},-\omega)\}$

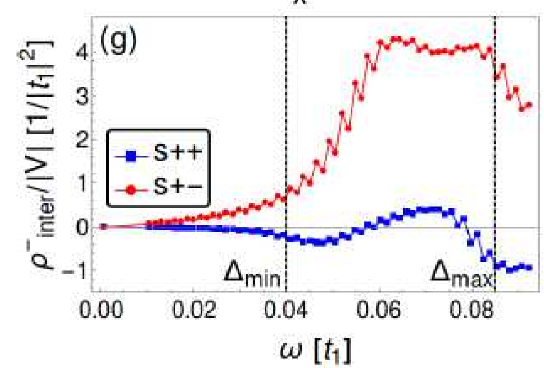












Single impurity (centered!) → robust against impurity potential

multiple impurities, dirty limit
→ Cherbychev BdG

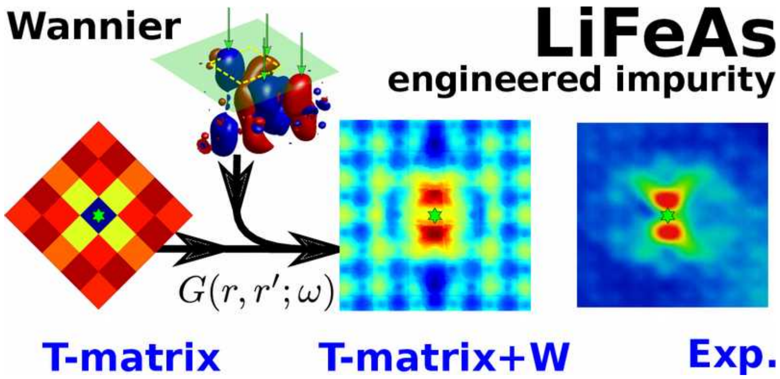
Summary

- Wannier method: basis transformation of the lattice Green function
- Qualitative correct (symmetry) and quantitative predictive results
- inelastic tunneling

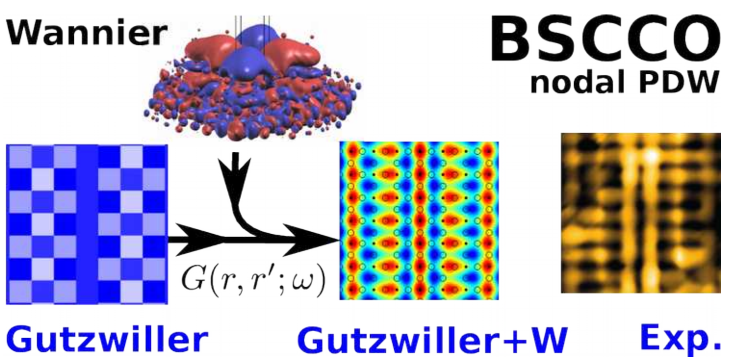
S. Chi, (…) AK, et al., arXiv:1703.07002

- sign change of order parameter

Martiny, Kreisel, Hirschfeld, Andersen
arXiv:1703.04891

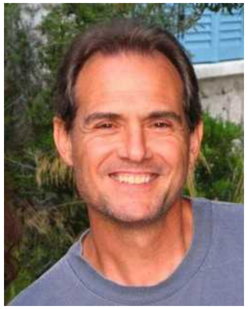


S. Chi, (...) , **A. Kreisel**, *et al.* Phys. Rev. B **94**, 134515 (2016)
A. Kreisel, *et al.* Phys. Rev. B **94**, 224518 (2016)



Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey et al., New J. Phys. **19**, 013028 (2017)

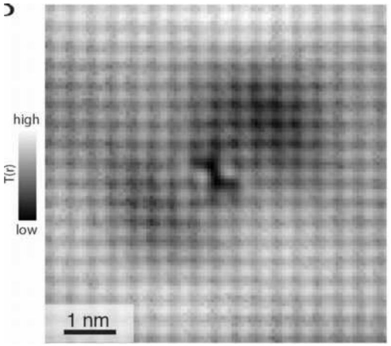
Acknowledgments



Measurement+modelling

- Problem: shift theorem in FT → single impurity (centered)

$$\rho_-(\vec{q},\omega) = Re\{g(\vec{q},+\omega)\} - Re\{g(\vec{q},-\omega)\}$$



- Theory:
  use measured gap
  +electronic structure

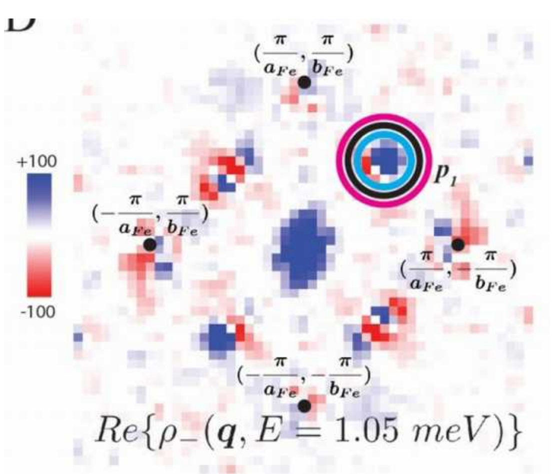
$$G_{k,k'}(\omega) = G^0_{k-k'}(\omega) + G^0_k(\omega)T(\omega)G^0_{k'}(\omega)$$

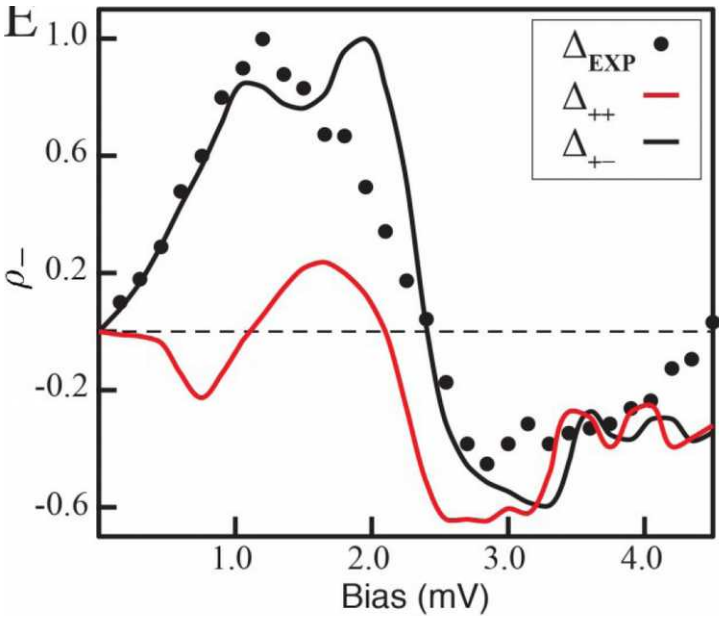
$$T(\omega) = \left[1 - V_{imp}G_0(\omega)\right]^{-1}V_{imp}$$

$$\delta N(\boldsymbol{q},\omega) = \frac{1}{\pi}Tr\{Im\sum_k G^0_k(\omega)T(\omega)G^0_{k+q}(\omega)\}$$

$$\rho(\omega) = \sum'_q \delta N(\boldsymbol{q},\omega)$$

- separate interband scattering contributions





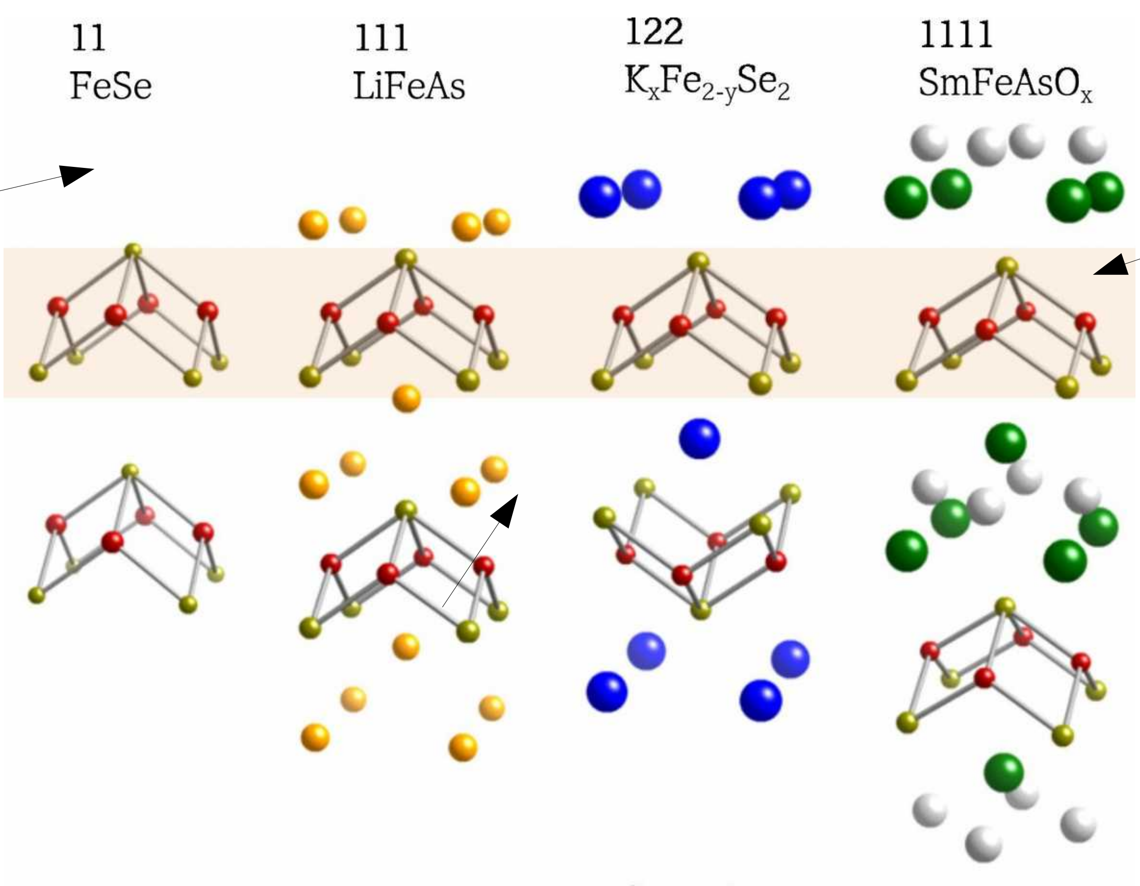
→ no sign change in signal, thus GAP changes sign

Layered superconductors

LDOS of sample at given energy at the tip position

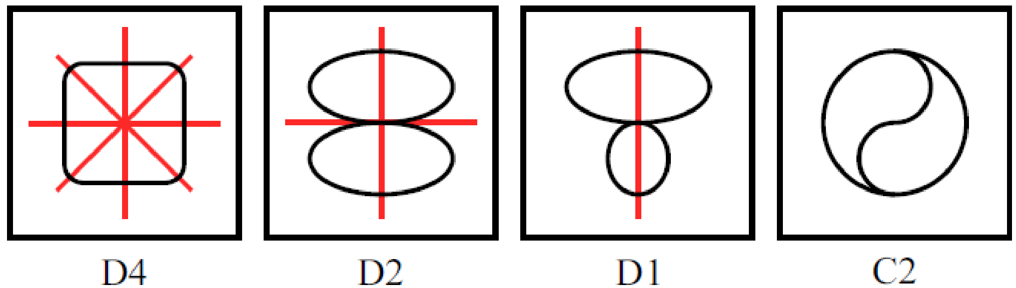
- Iron based superconductors

surface termination:
Se (FeSe)
Li (LiFeAs)

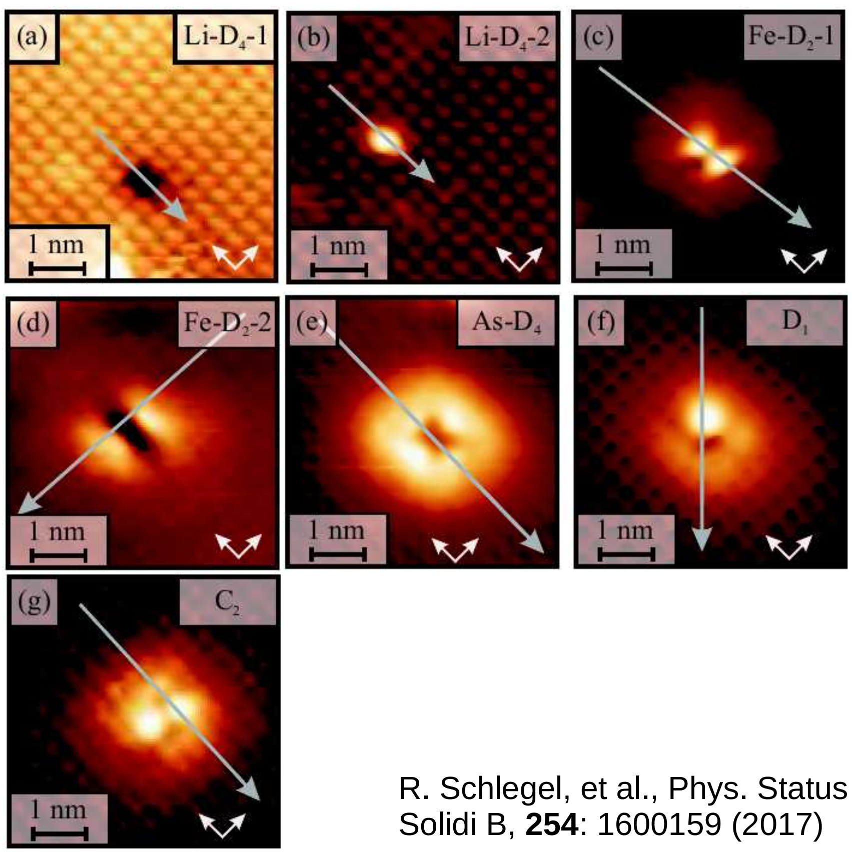


common layer: states at the Fermi level

LiFeAs: other native impurities

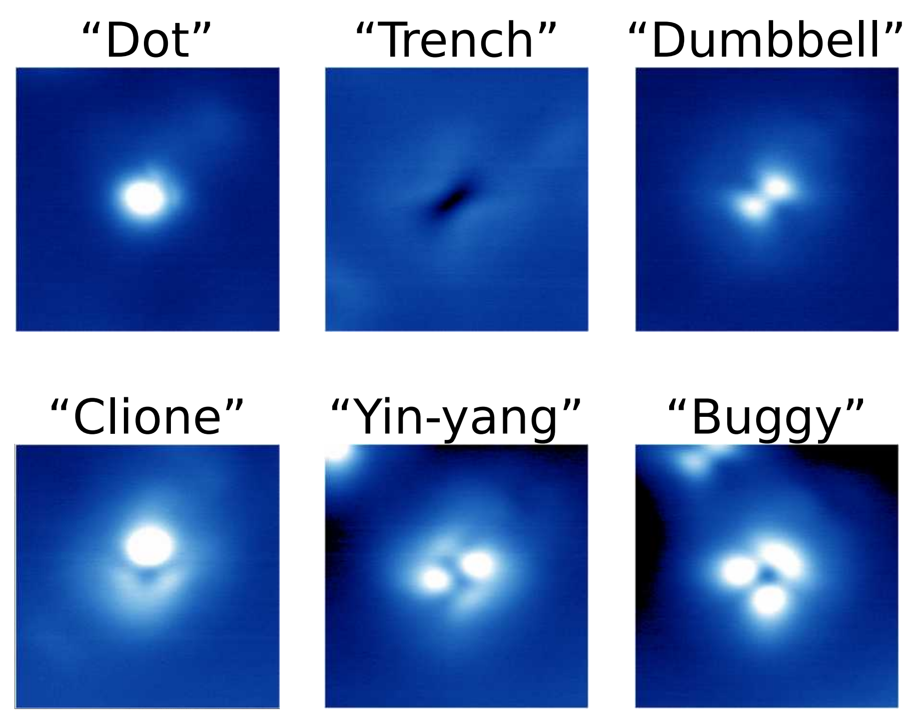


Schönflies classification of impurities



R. Schlegel, et al., Phys. Status Solidi B, **254**: 1600159 (2017)

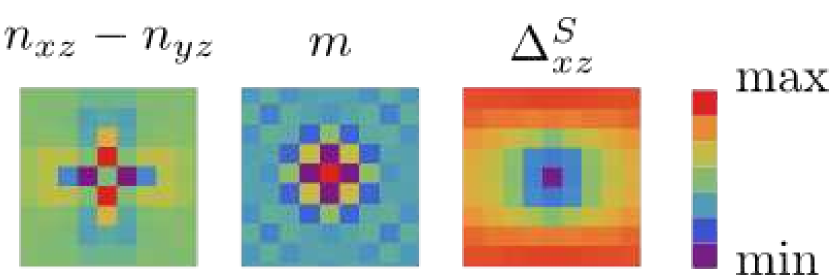
Hanaguri, unpublished (KITP 2011)



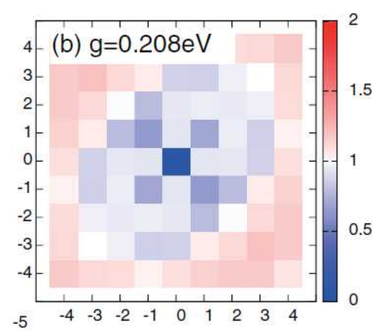
Chiral defects

- from a symmetry perspective not compatible to impurities on any single site in LiFeAs
- multiple impurities?
- local order?

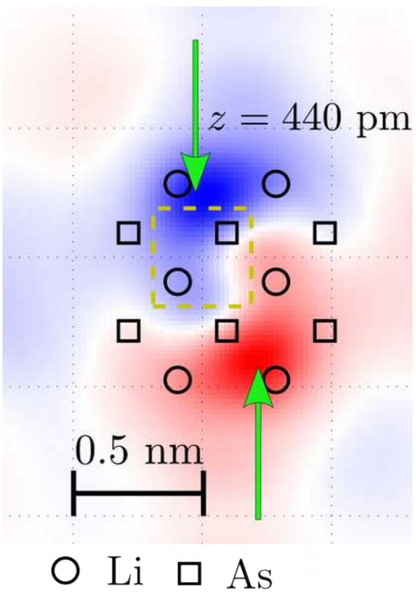
local orbital order
+ Wannier function
→ chiral defect structure



Gastiasoro, Andersen, J. Supercond Nov. Magn., **26**, 2651 (2013)



Inoue, Yamakawa, Kontani PRB 85, 224506 (2012)



d_xz Wannier function on Fe(2)