Towards a realistic simulation of disorder in unconventional superconductors

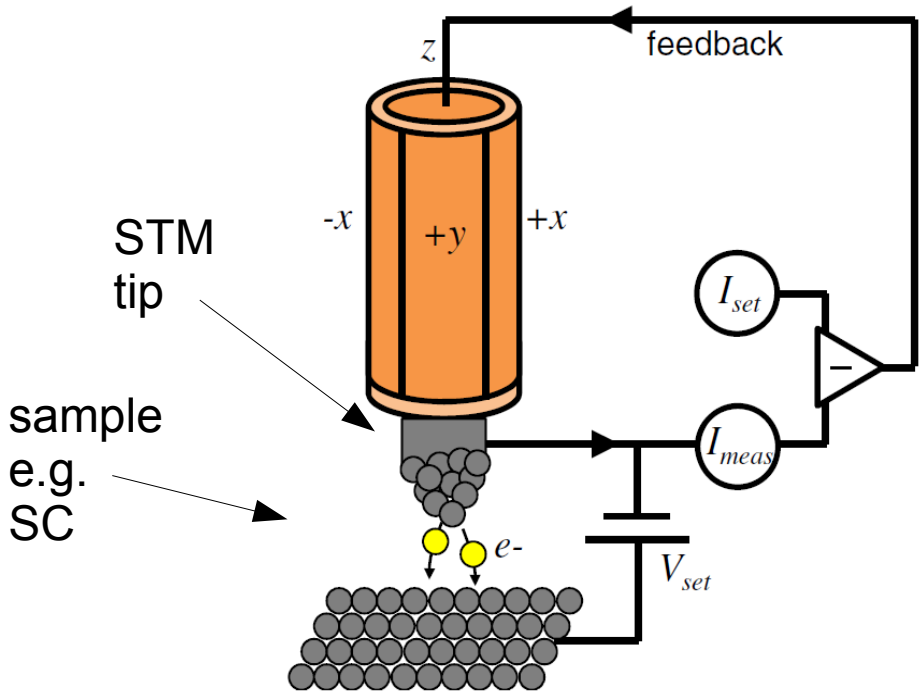
Andreas Kreisel, Brian Andersen
Niels Bohr Institute, University of Copenhagen, 2100 København, Denmark
Peayush Choubey, Peter Hirschfeld
Department of Physics, University of Florida, Gainesville, FL 32611, USA
Tom Berlijn
Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
Wei Ku
Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA

Phys. Rev. B **90**, 134520 (2014)
Phys. Rev. Lett. **114**, 217002 (2015)
arXiv:1607.03192

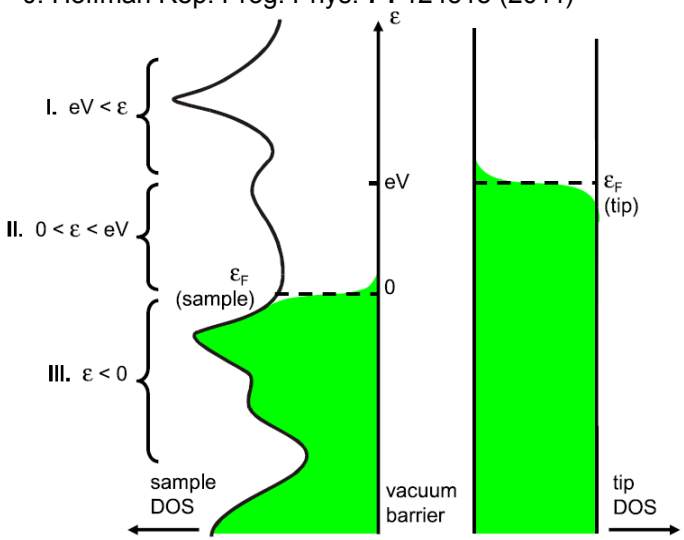
Outline

- Motivation
  - STM: impurities as probe for electronic structure, order parameter
  - layered superconductors, complications
- Theoretical methods to investigate impurity physics in superconductors
- Using wavefunction information in layered superconductors
- Applications
  - BiSrCaCuO (single band, d-wave)
  - LiFeAs (multiband, s-wave)

Scanning tunnelling microscopy



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



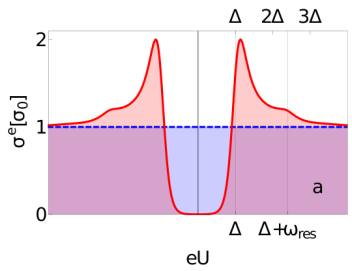
Inelastic tunneling:
coupling to bosonic mode

Tunnelling current:

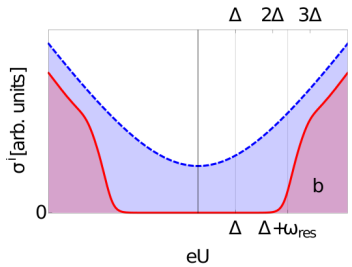
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

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

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



superconducting state



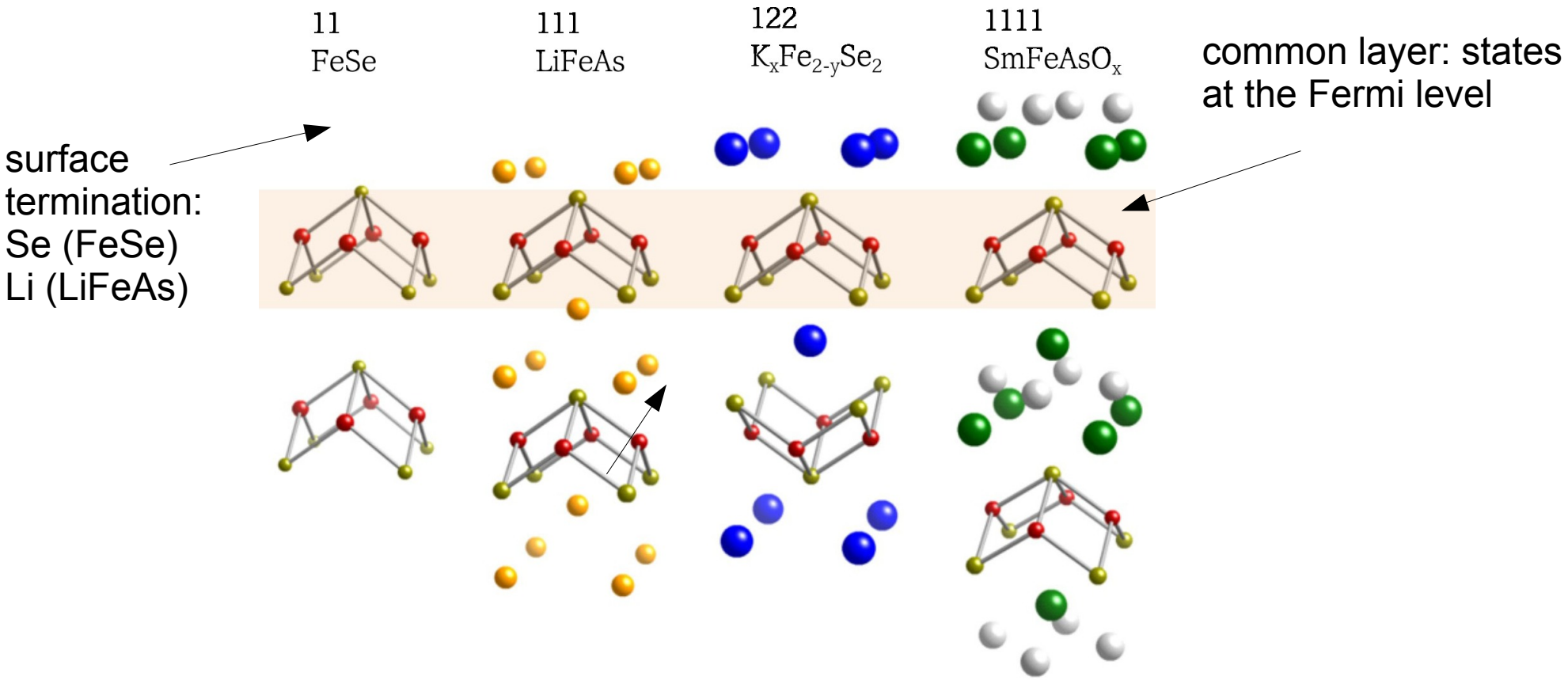
normal state

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)

Layered superconductors

LDOS of sample at given energy at the tip position

- Iron based superconductors



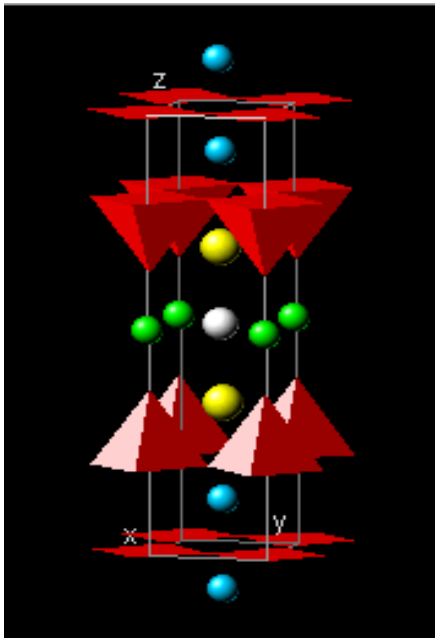
Layered superconductors

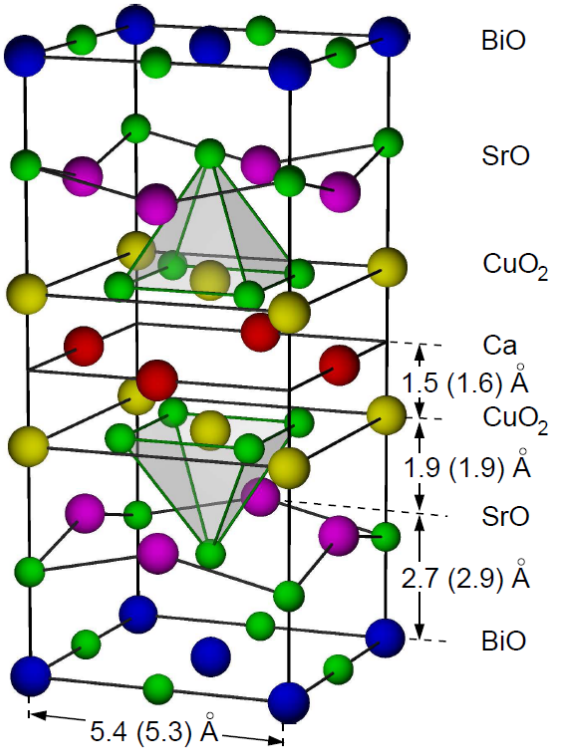
- Cuprates

Hg1Ba2Ca2Cu3O8

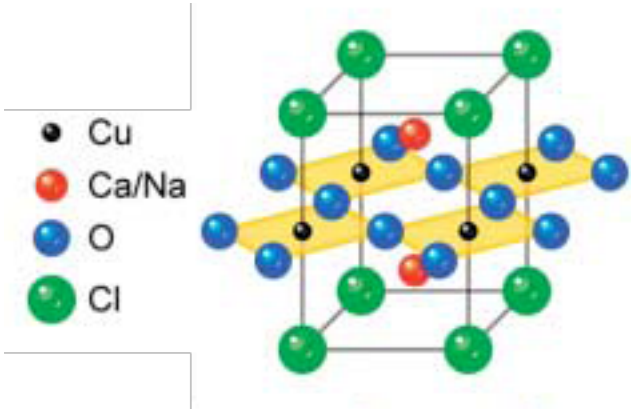
Tc = 135 K
under pressure: 153 K

Cu/O





Bi-2212

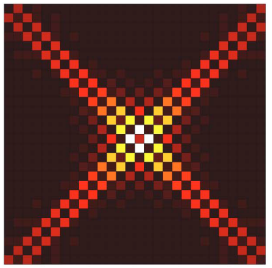


Na-CCOC

Bound states of nonmagnetic impurity

- d-wave superconductors
  - local LDOS: 4 fold pattern

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



  - low energy bound state

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

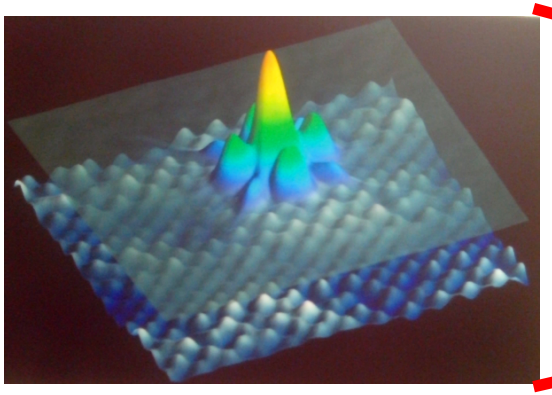
A. V. Balatsky, M. I. Salkola, and A. Rosengren
Phys. Rev. B **51**, 15547 (1995)

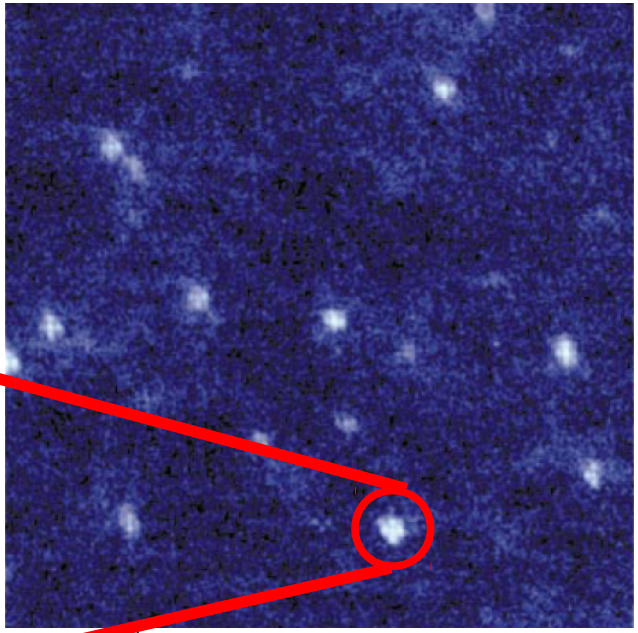
Stamp, Journal of Magnetism and Magnetic Materials, **63**, 429 - 431 (1987) (p-wave)

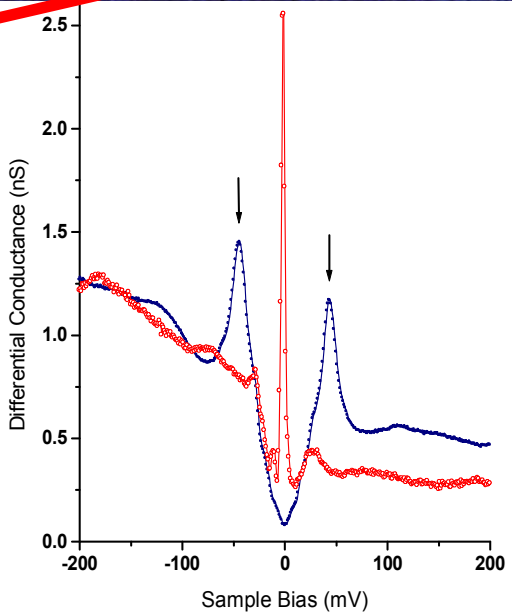
STM experiment on Bi-2212

- LDOS map at -1.5 meV
  ~20 Zn atoms in field of view
  - 4 fold pattern

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

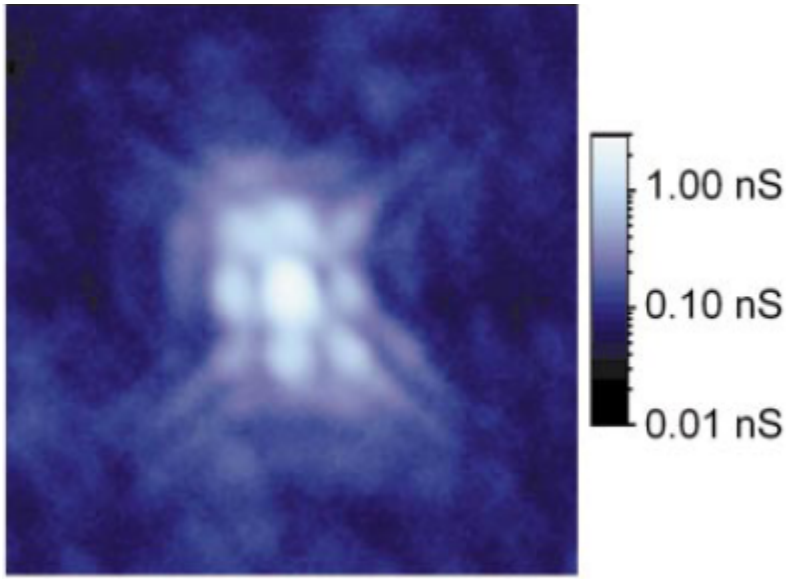


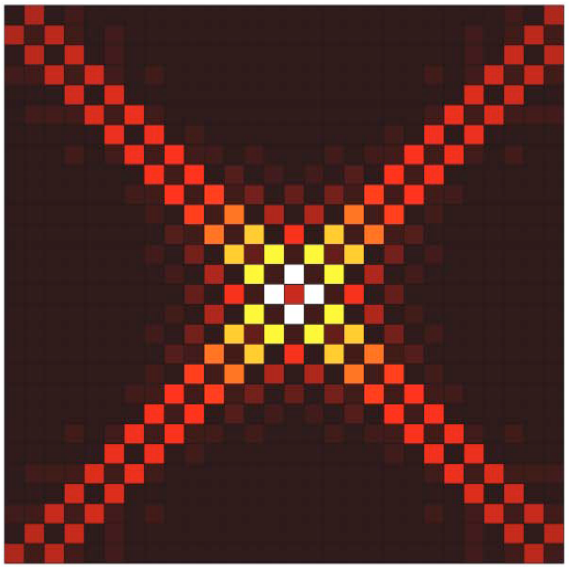




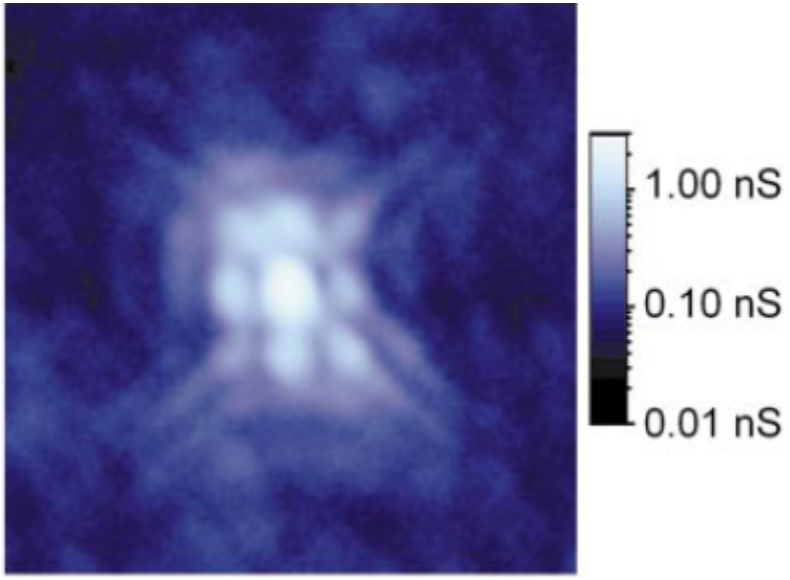
  - low energy bound state
    in on site spectrum

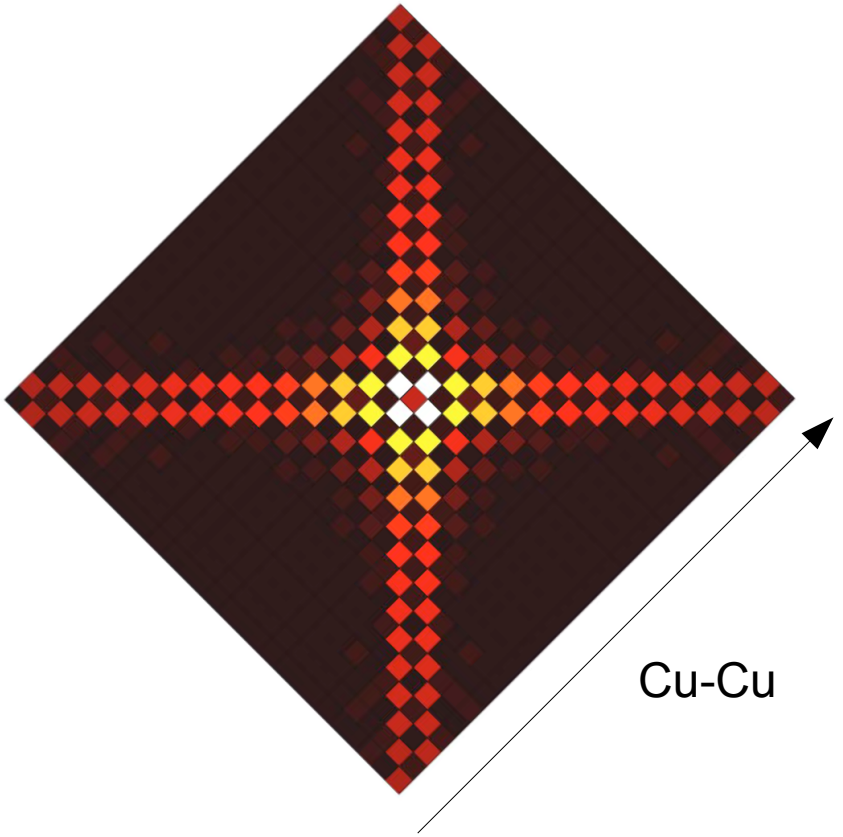
comparison to theory

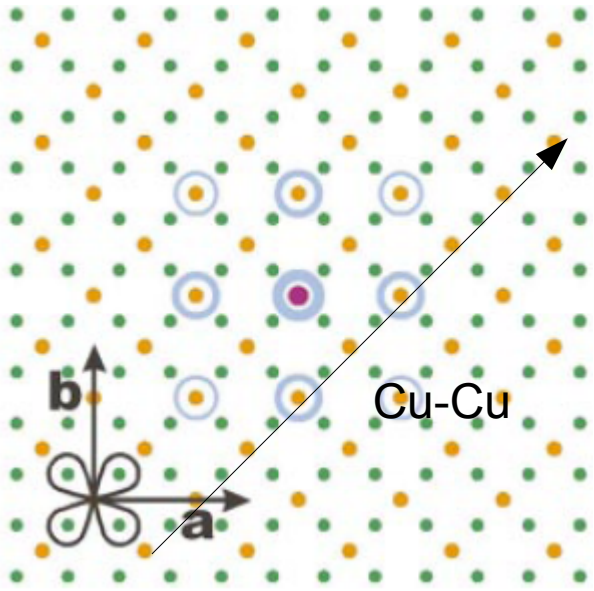




comparison to theory





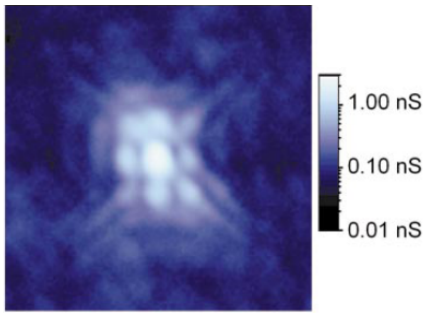


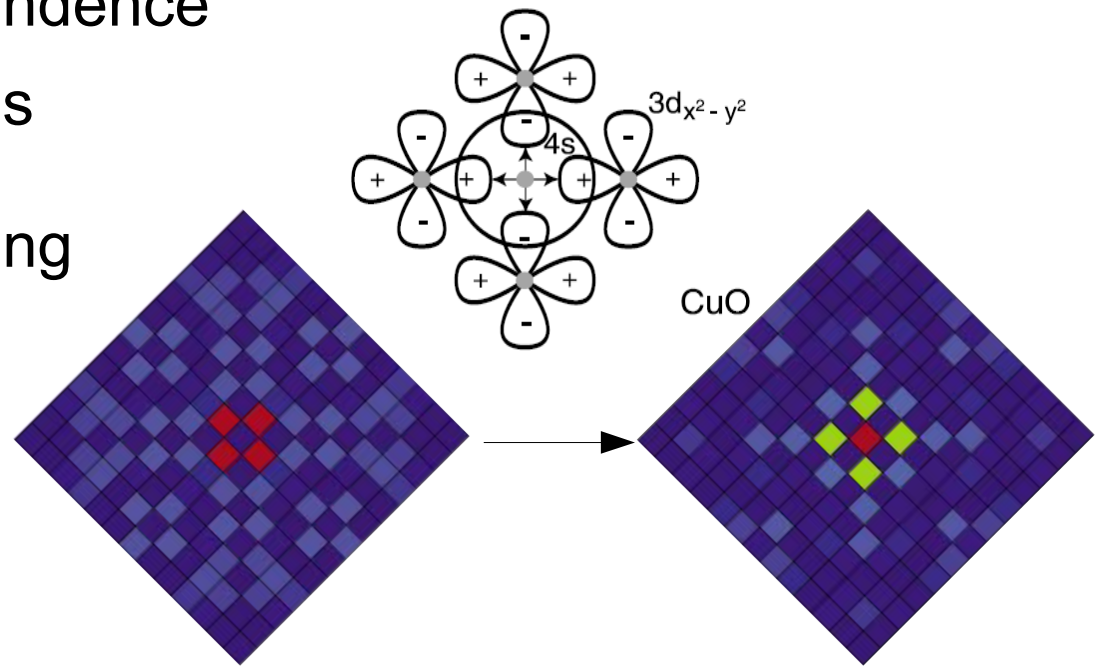
Theories for spatial pattern

- extended impurity potentials (magnetic Ni impurity)
- Correlations: “Kondo screening” (magnetic impurity), “modifications of the theory for the case of a nonmagnetic impurity” → consistent with experimental spatial dependence
- Bi-O filter function: STM probes neighbouring Cu states due to momentum dependent tunnelling matrix elements

Jian-Ming Tang and Michael E. Flatté PRB **66**, 060504(R) (2002)

Anatoli Polkovnikov PRB **65**, 064503 (2002)





Martin *et al.*, PRL **88**, 097003 (2002)

Theory: State of the art methods

- Hamiltonian

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

band structure
kinetic energy

$$H_0 = \sum_{\mathrm{R\,R'},\sigma} t_{\mathrm{R\,R'}} c^{\dagger}_{\mathrm{R}\,\sigma} c_{\mathrm{R'}\,\sigma} - \mu_0 \sum_{\mathrm{R},\sigma} c^{\dagger}_{\mathrm{R}\,\sigma} c_{\mathrm{R}\,\sigma}$$

superconductivity
gap function / pairing

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

impurity scatterer
(non)magnetic
potential / T_2 scatterer

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

- T-matrix calculations
- self-consistent mean field theory (BdG)
- lattice Green function

$$\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}_0(\mathbf{r}-\mathbf{r}',\omega) + \hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r}',\omega)$$

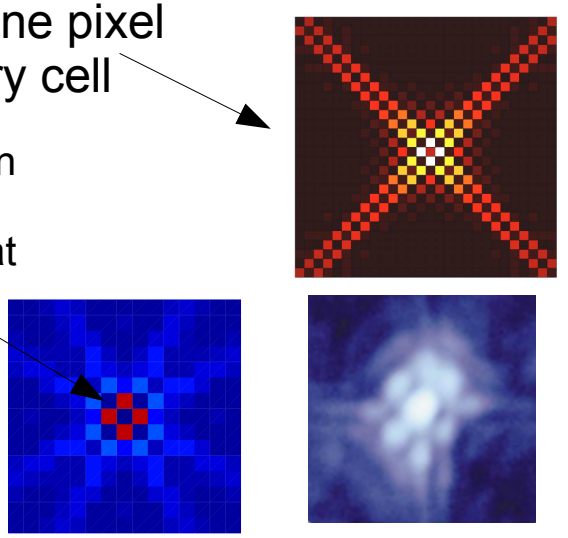
- Local Density of States (LDOS)

$$N_{\mathrm{imp}}(\mathbf{r},\omega) = -\frac{1}{\pi}\,\mathrm{Im}[\hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r},\omega)]_{11}$$

Zn impurity in BiSrCaCuO

"resolution": one pixel per elementary cell

minimum on impurity, maximum at NN



T-matrix calculation
Bi-O filter function needed

experiment

Martin *et al.*, PRL **88**, 097003 (2002)

Theory: State of the art methods Bogoliubov-de Gennes (BdG)

- Hamiltonian $H = H_0 + H_{\mathrm{BCS}} + H_{\mathrm{imp}}$
- self-consistent solution in real space (NxN grid, determine gaps) $\Delta_{\mathrm{R\,R'}} = \Gamma_{\mathrm{R\,R'}} \langle c_{\mathrm{R'}\downarrow} c_{\mathrm{R}\uparrow} \rangle$
- eigenvalues E_n, eigenvectors (u_n, v_n)
- lattice Green function

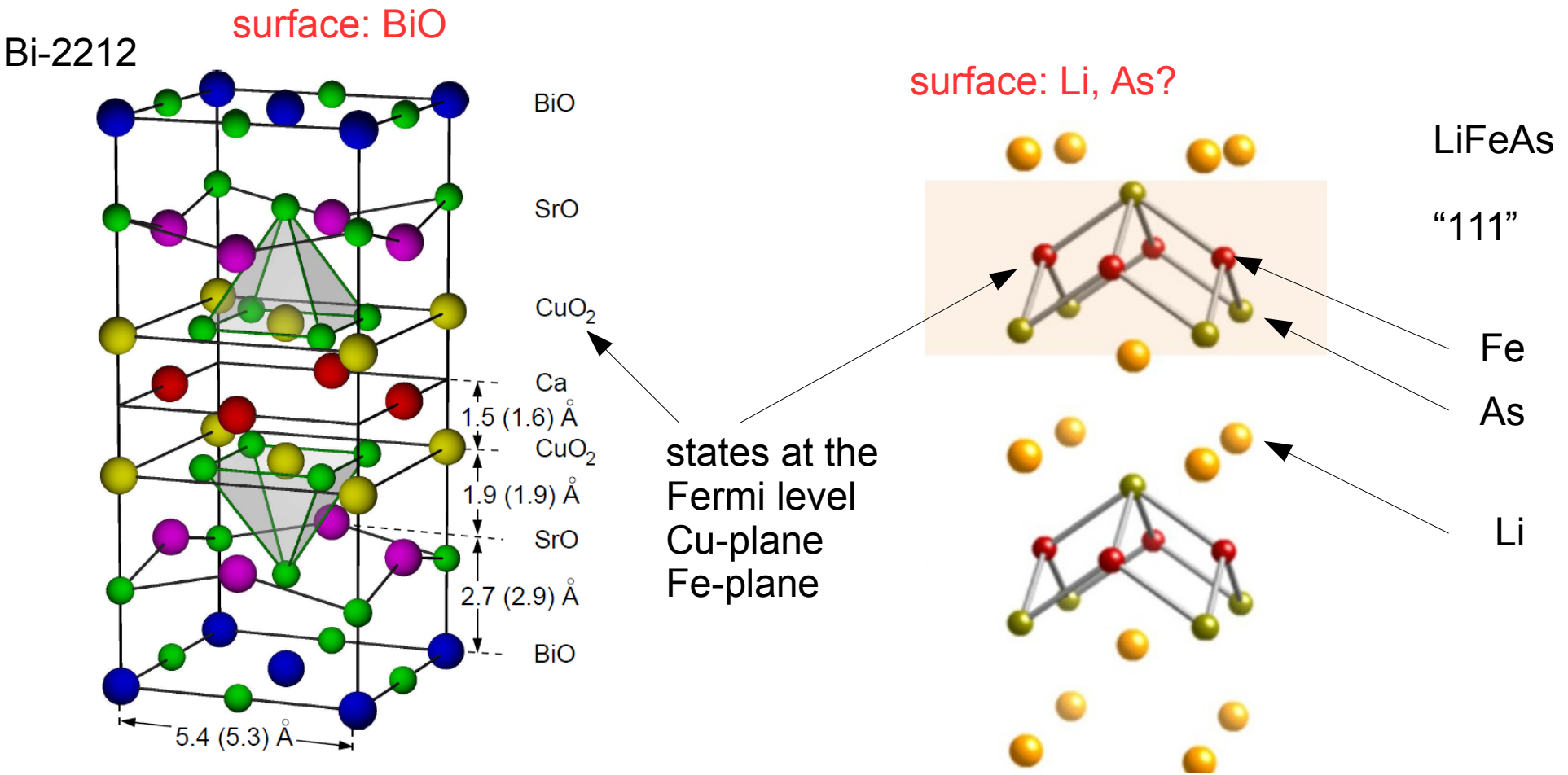
$$G_\sigma(\mathrm{R}, \mathrm{R'}; \omega) = \sum_n \left(\frac{u_{\mathrm{R}}^{n\sigma} u_{\mathrm{R'}}^{n\sigma *}}{\omega - E_{n\sigma} + i0^+} + \frac{v_{\mathrm{R}}^{n-\sigma} v_{\mathrm{R'}}^{n-\sigma *}}{\omega + E_{n-\sigma} + i0^+} \right)$$

Layered superconductors

- 2 examples: surface atoms ≠ superconducting layer

Cuprates

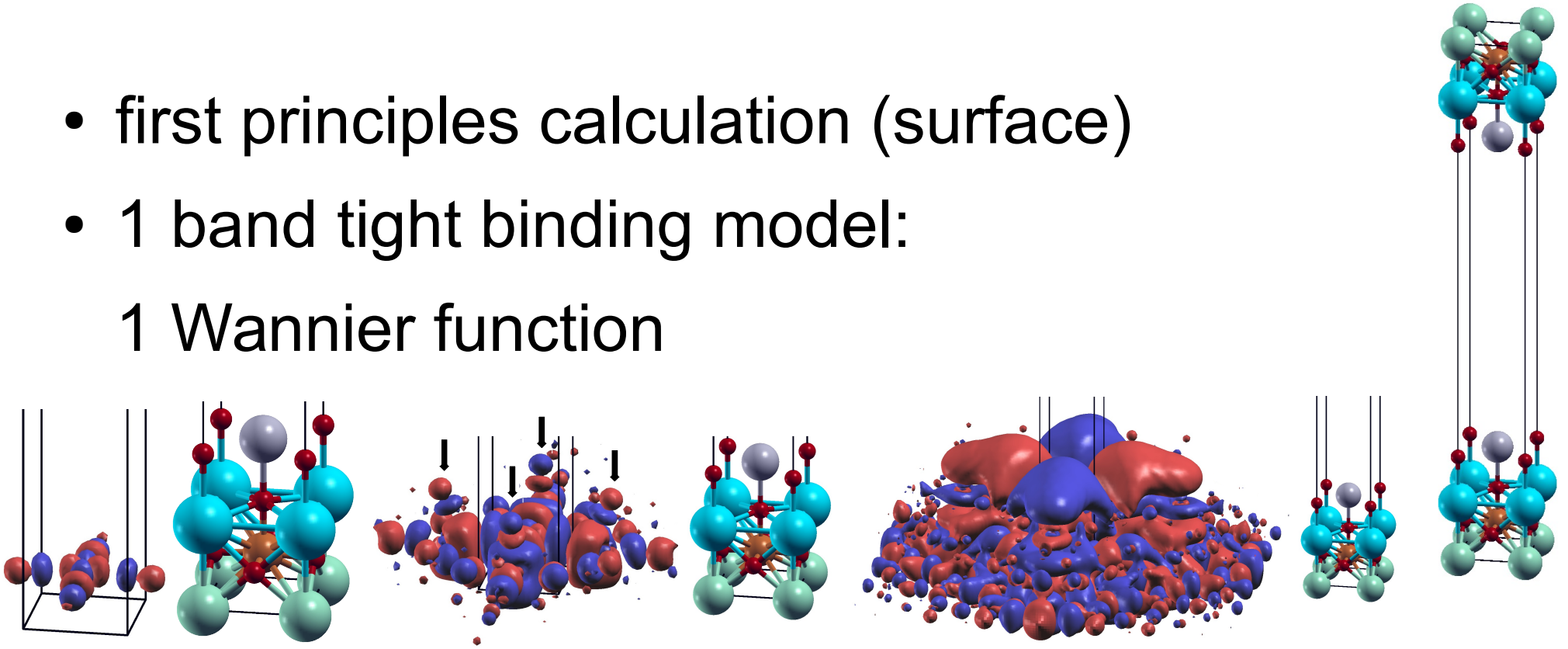
Iron based superconductors



Wannier method

- first principles calculation (surface)
- 1 band tight binding model:

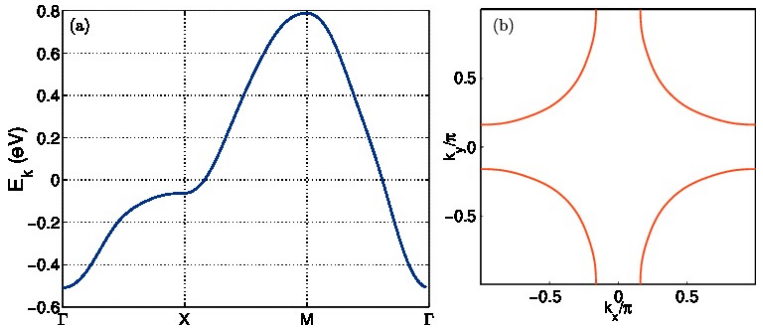
  1 Wannier function

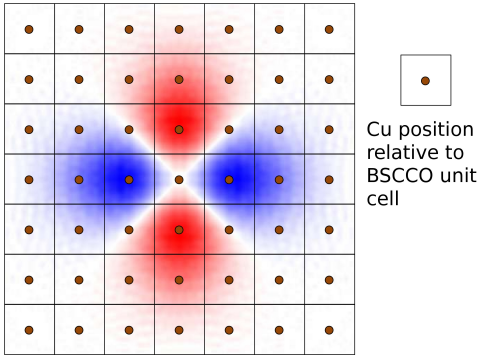


Cu dxy

NN apical O tails

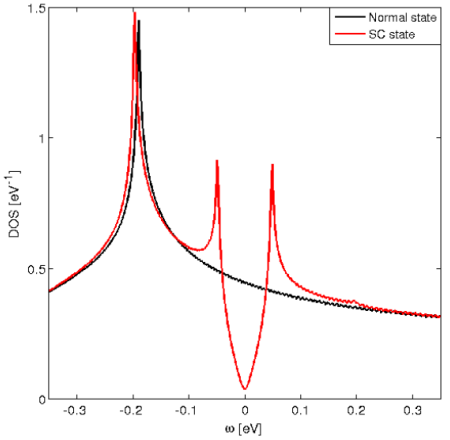
at surface: only contributions to NN





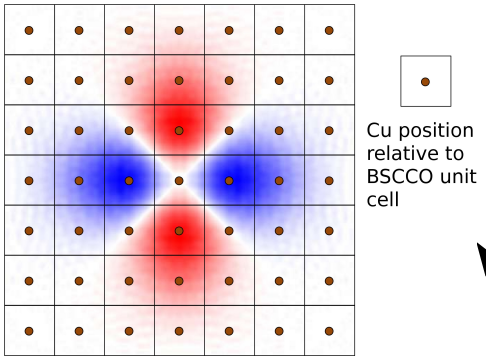
Superconductivity

- superconducting order parameter (d-wave) (phenomenology or calculation fx. mean-field)



- continuum Green function

$$\psi_\sigma(\mathsf{r}) = \sum_{\mathsf{R}\,\mu} c_{\mathsf{R}\,\mu\sigma} w_{\mathsf{R}\,\mu}(\mathsf{r})$$



surface Wannier function with phases

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

continuum position

nonlocal contributions

lattice Green function

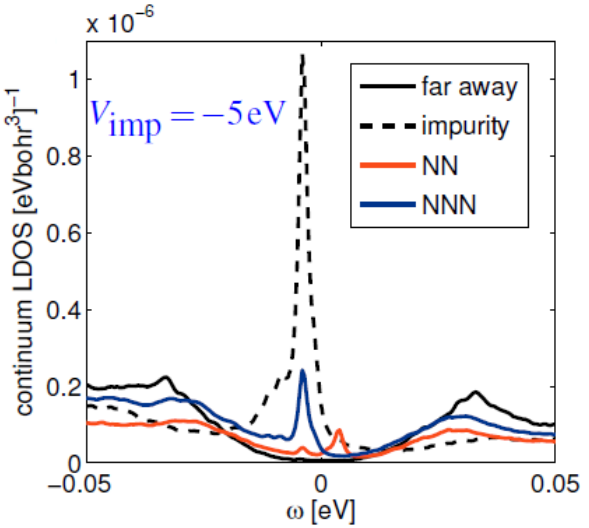
local density of states (LDOS)

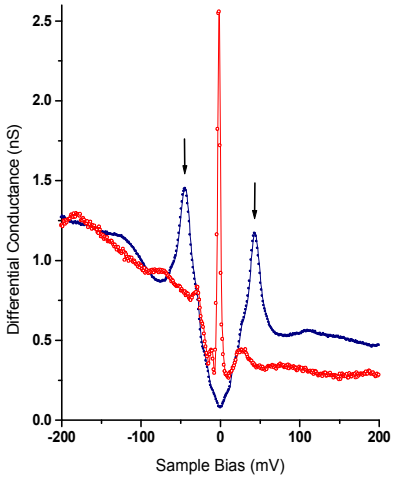
$$\rho(\mathsf{r},\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,G(\mathsf{r},\mathsf{r};\omega)$$

BSCCO: Results
STM maps and spectra

- d-wave order parameter
- Zn impurity:
  V_{imp}=-5 eV
  resonance: -3.6 meV

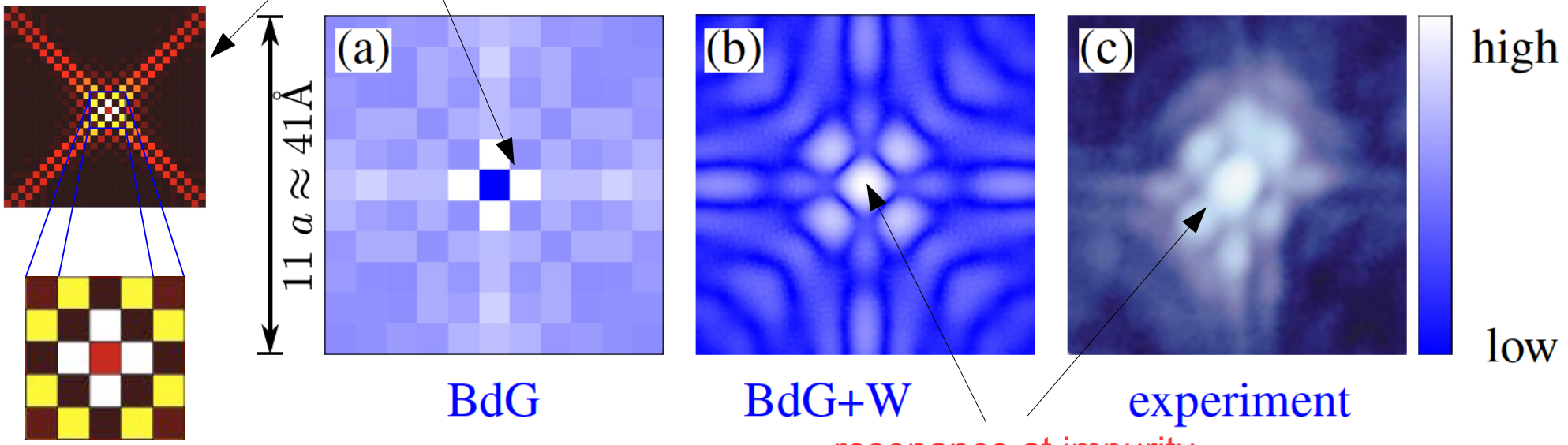
Pan et al., Nature **403**, 746 (2000)



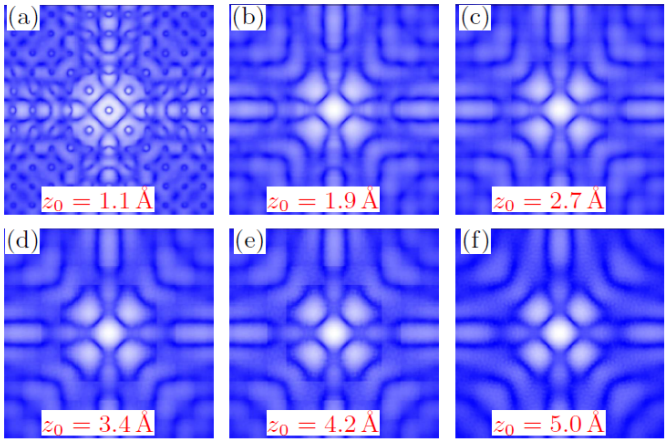


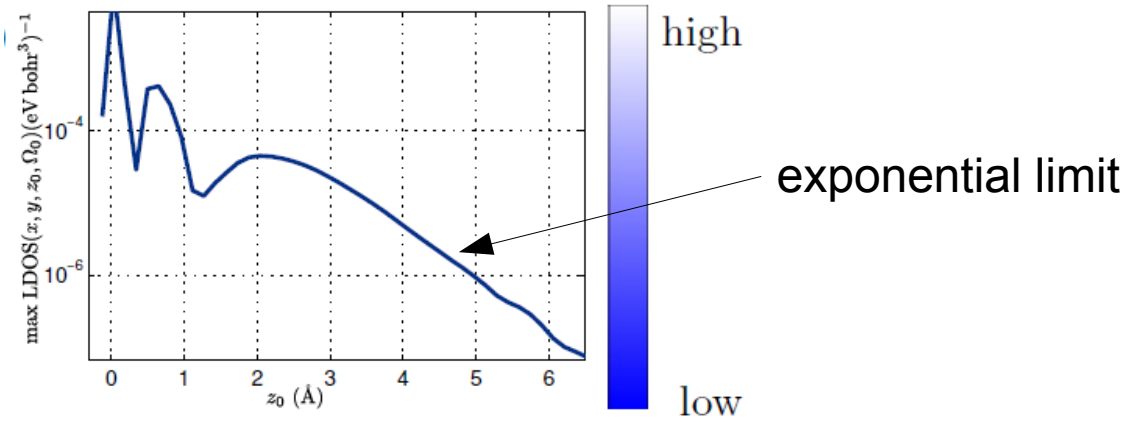
Zhu *et al.*, PRB **67**, 094508 (2003)

resonance at NN

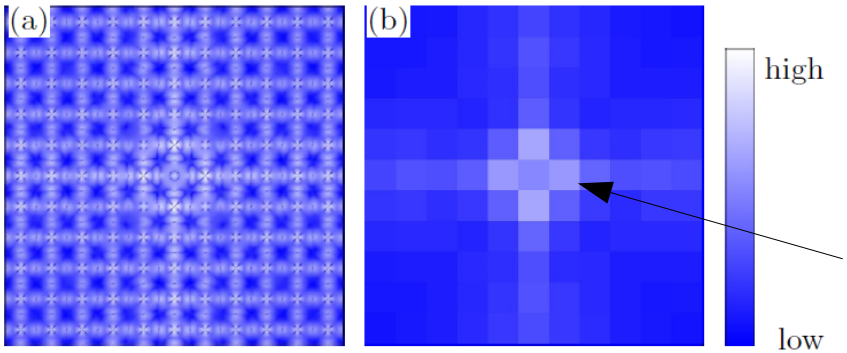


- dependence on tip height

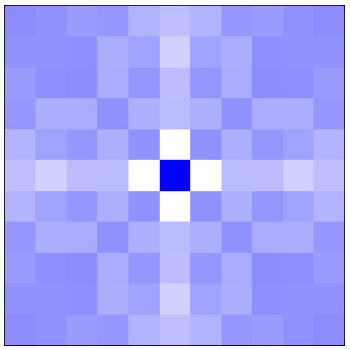




- continuum LDOS in the Cu-plane

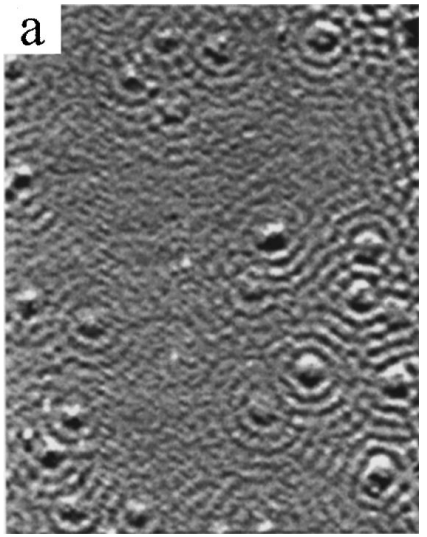


convolution with Gaussian blur
of 1 pixel per elementary cell



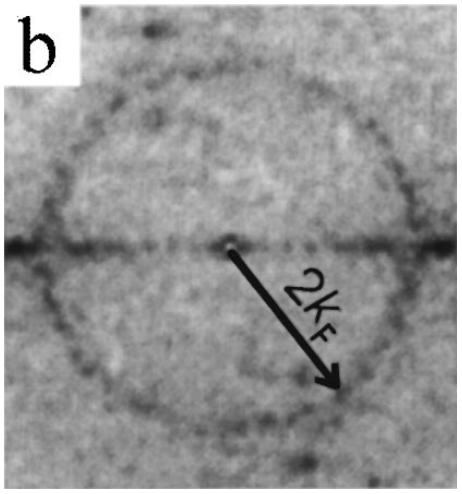
Quasiparticle Interference (QPI)

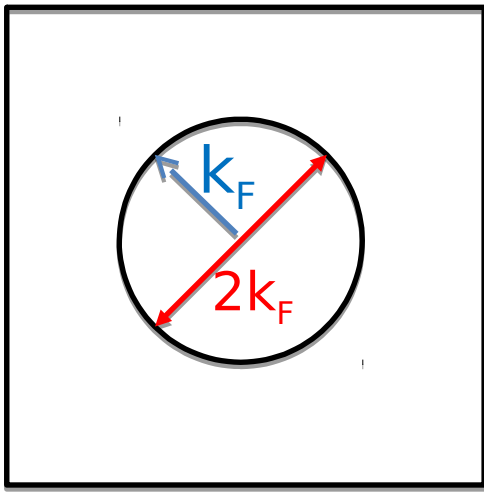
- STM on normal metal (Cu)
  - impurities
  - Friedel oscillations



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

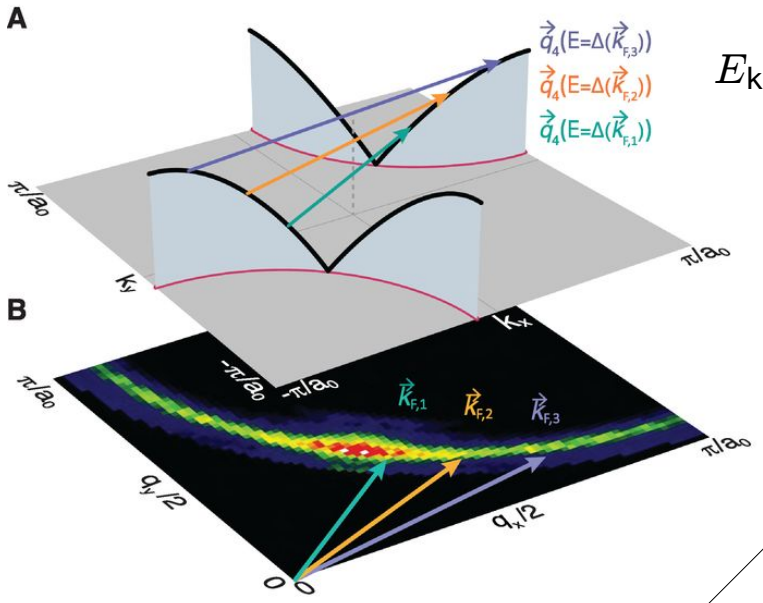
- Fourier transform of conductance map
  - mapping of constant energy contour





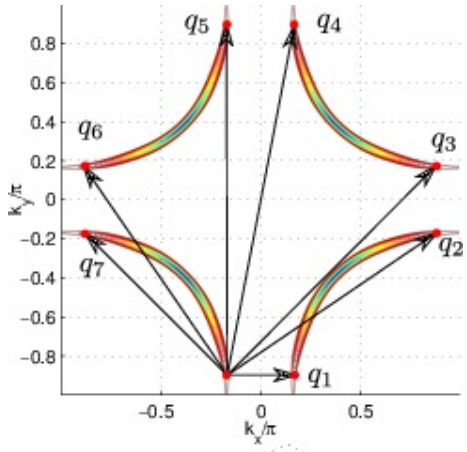
QPI in superconductors

- Fourier transform of differential conductance maps

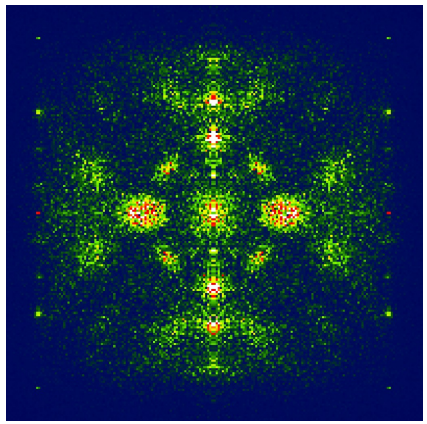


$$E_k = \pm\sqrt{\epsilon_k^2 + \Delta_k^2}$$

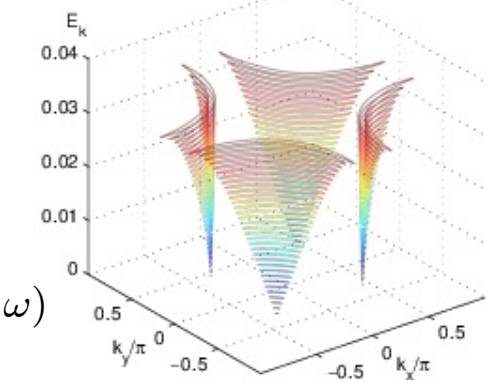
energy integrated maps: trace back Fermi surface



FT of conductance map at +22 meV



$$\Lambda(q) = \int_0^{\Delta_0} d\omega\, Z(q,\omega)$$



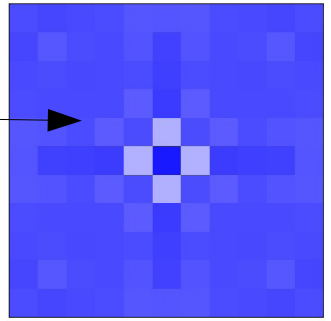
K Fujita et al. Science **344**, 612 (2014)

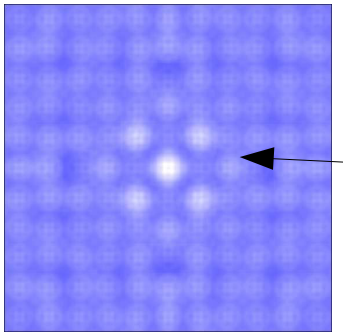
octet model: 7 scattering vectors between regions of high DOS

Quasi Particle Interference (QPI)

- Fourier transform of conductance maps
- BSCCO: weak potential scatterer

no intra-unitcell information
1 pixel per elementary cell

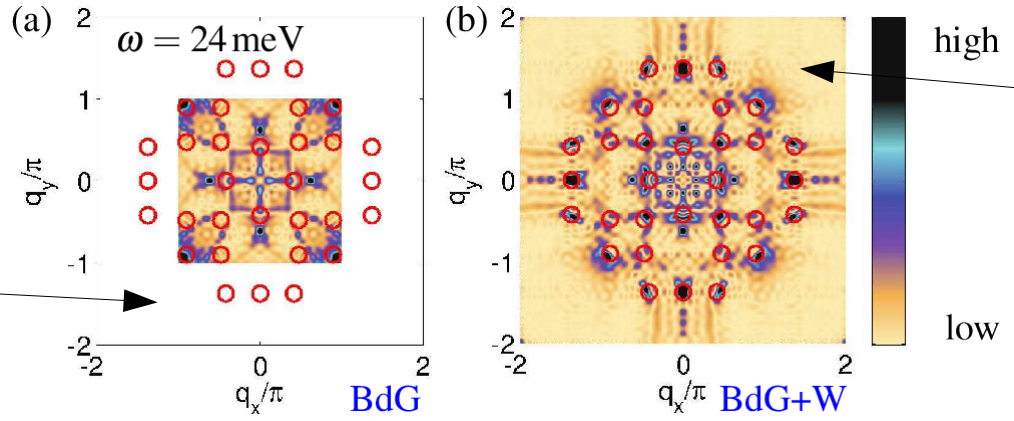




atomic scale local density of states at STM tip position

full information for all scattering vectors

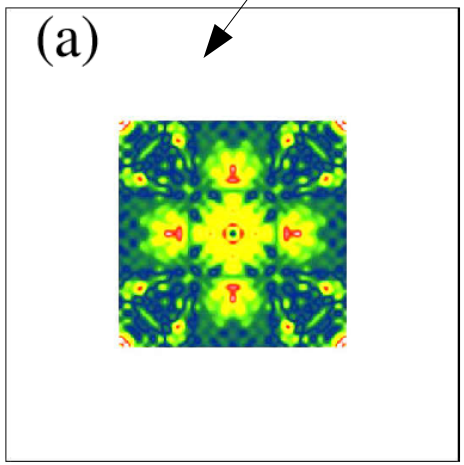
no information beyond first BZ

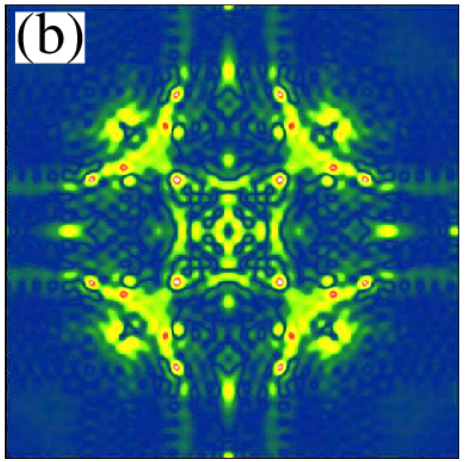


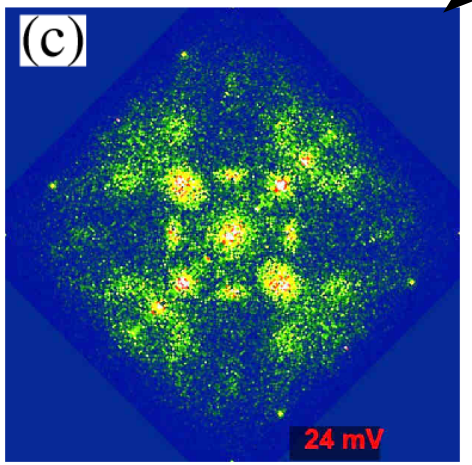
Comparison to experiment

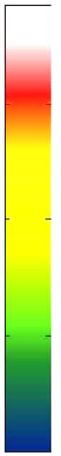
no large q information

$$Z(r,\omega) = \frac{g(r,\omega)}{g(r,-\omega)} = \frac{\rho(r,\omega)}{\rho(r,-\omega)}$$





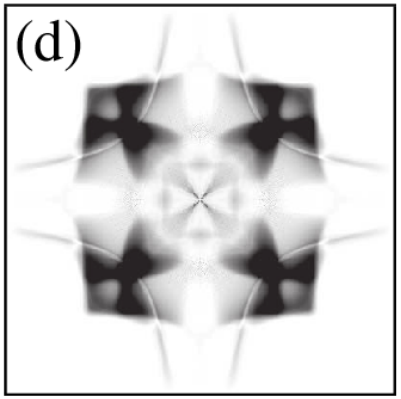


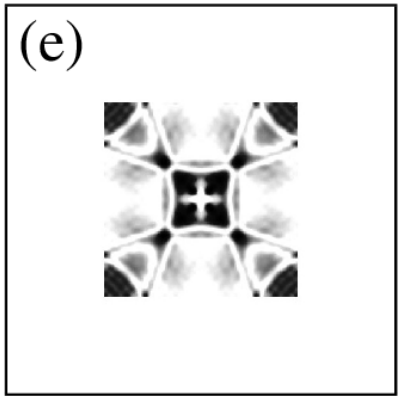


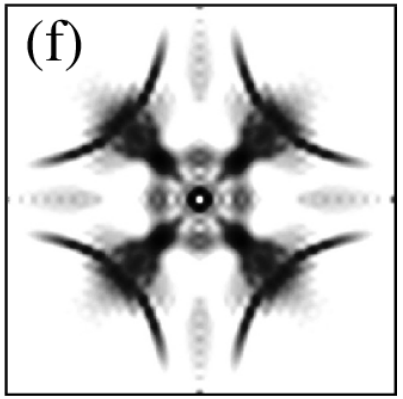
relative conductance map, Fourier transformation

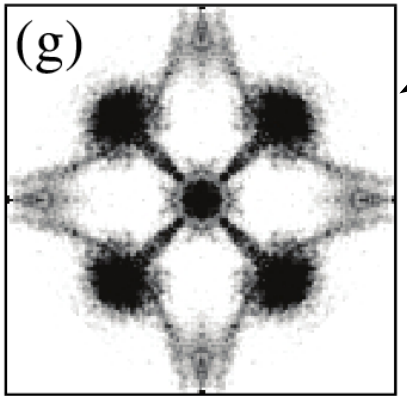
BdG | BdG+W | experiment

$$\Lambda(\mathbf{q}) = \int_0^{\Delta_0} d\omega\, Z(\mathbf{q},\omega)\,.$$









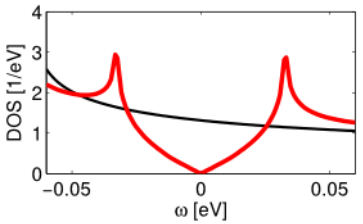
energy integrated relative conductance maps

T-matrix | BdG | BdG+W | experiment

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

Homogeneous superconductor

- phenomenological pairing interactions
  similar results from spin-fluctuation pairing



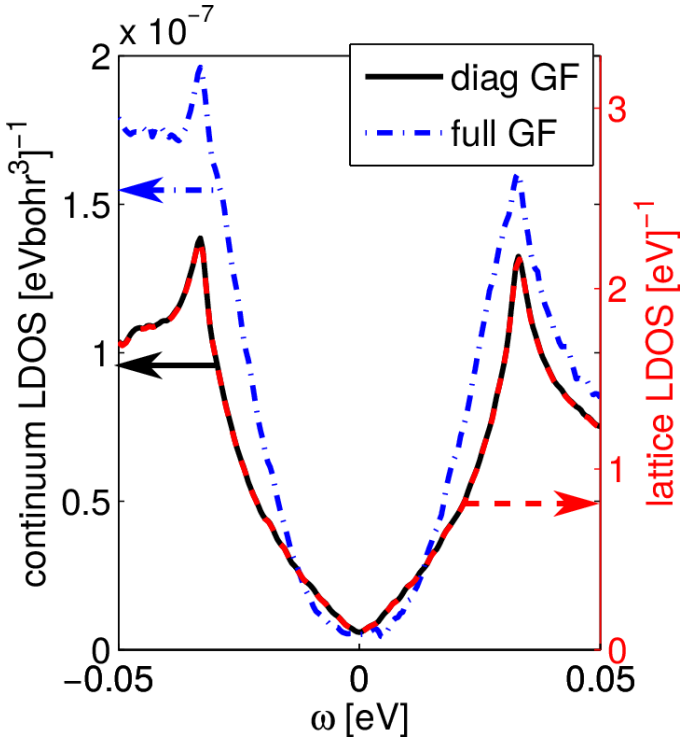
DOS of homogeneous superconductor

- spectra measured
  at the surface

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

local density of states (LDOS)

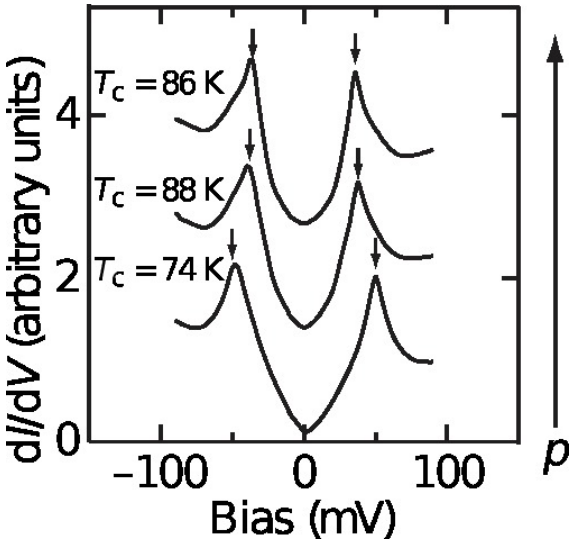
$$\rho(\mathsf{r}, \omega) \equiv -\frac{1}{\pi} \operatorname{Im} G(\mathsf{r}, \mathsf{r}; \omega)$$



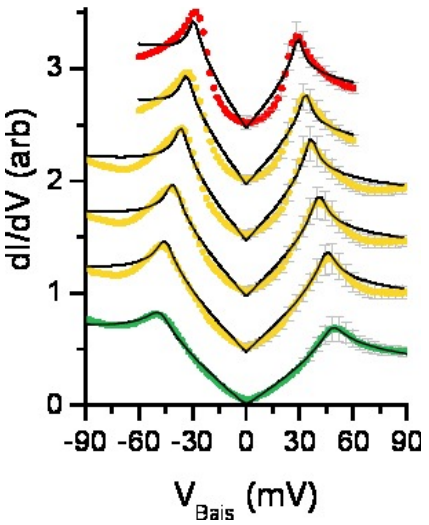
STM Spectra: homogeneous SC

- overdoped: U-shape, lower doping: V-shape

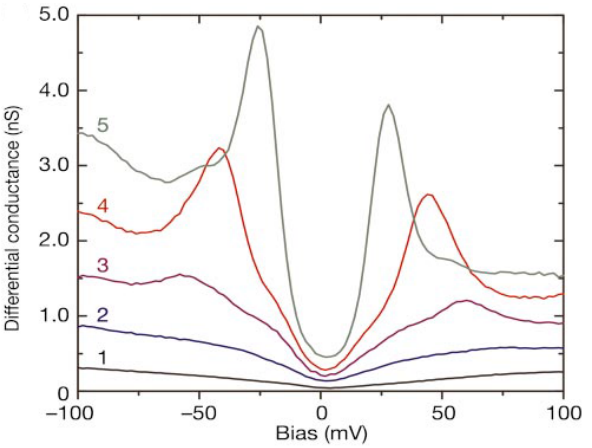
Kohsaka et al.
Nature, 454, 1072 (2008)

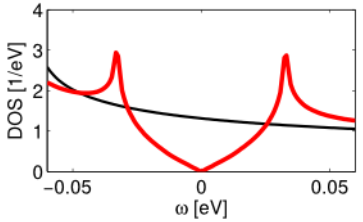


Alldredge et al.
Nature Physics, 4, 319 (2008)



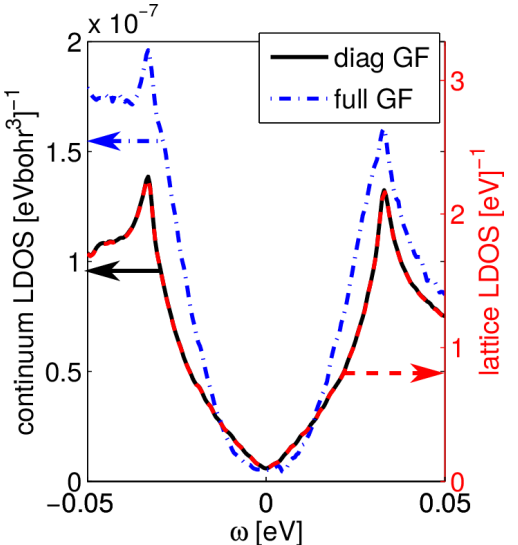
Pan et al. Nature, 413, 282 (2001)





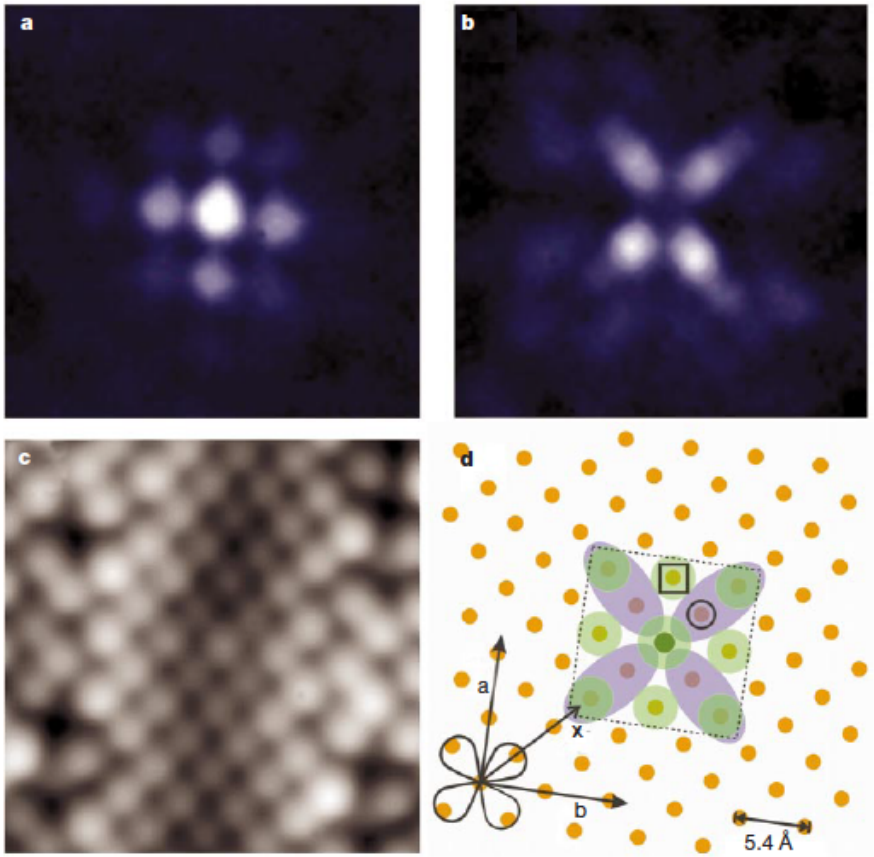
DOS of homogeneous superconductor

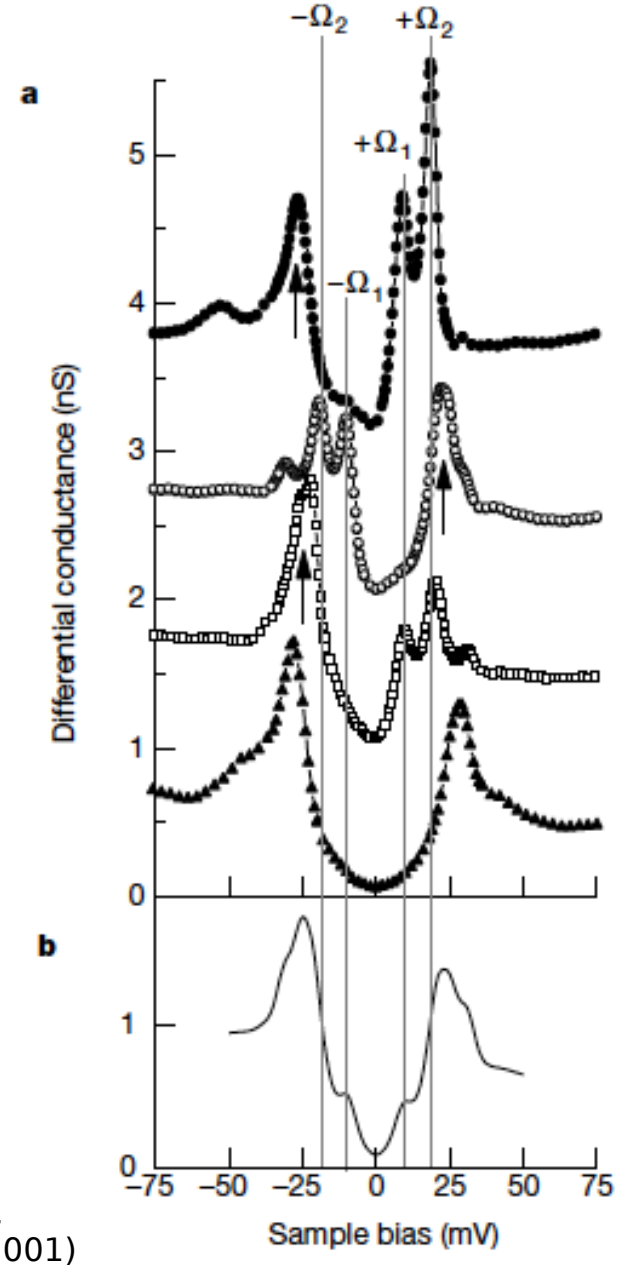
BdG+W: U shape enters natually within our method, applicable to overdoped regime



BSCCO: Magnetic impurity

- Ni on BSCCO:
  weak magnetic scatterer
- double resonance





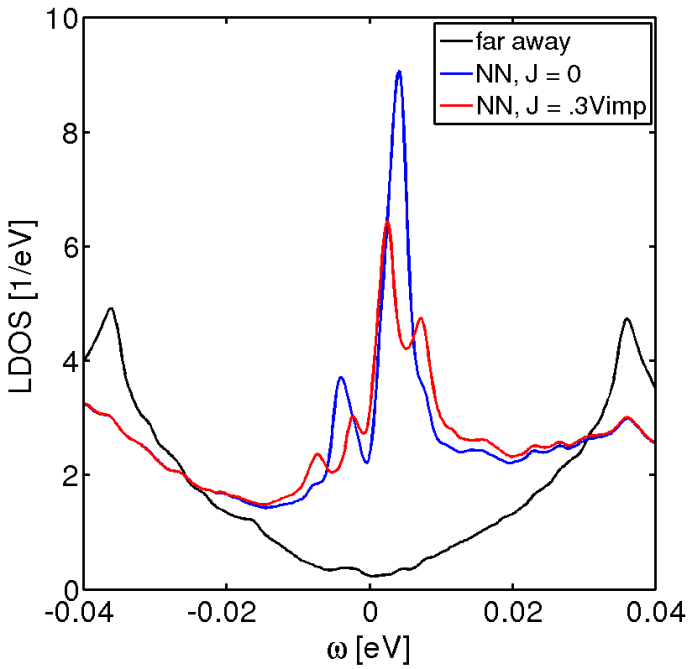
E. W. Hudson et al.,
Nature **411**, 920 (2001)

Ni impurity on BSCCO

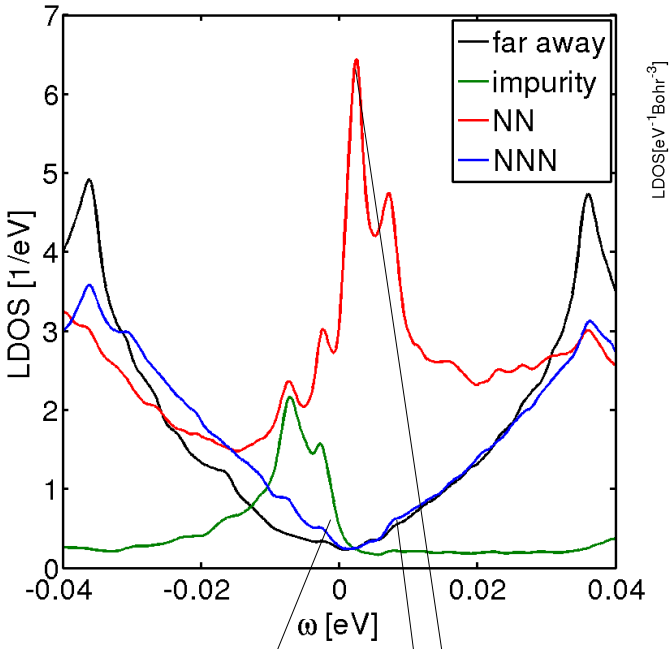
- chemistry: Ni 3d8 configuration → magnetic moment with S=1
- Classical spin: additional magnetic potential

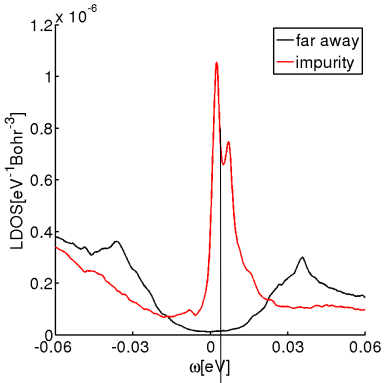
$$H_{\mathrm{imp}}^{\mathrm{mag}} = J(n_{\mathrm{R}\,*\uparrow} - n_{\mathrm{R}\,*\downarrow})$$

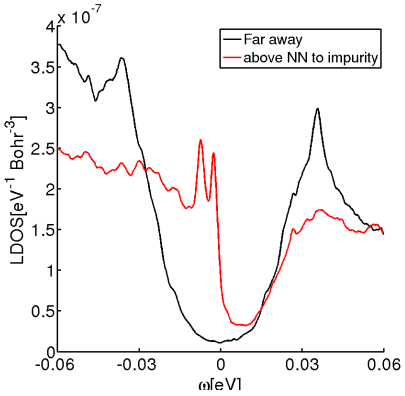
- resonances at
  +/- 2.4 meV (up)
  +/- 7.2 meV (down)

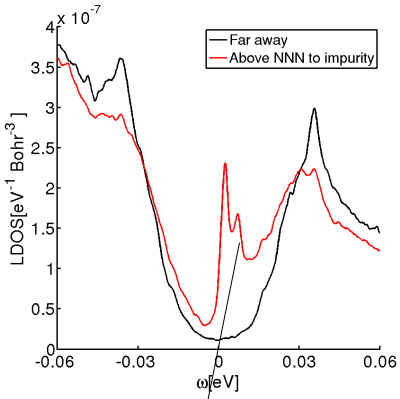


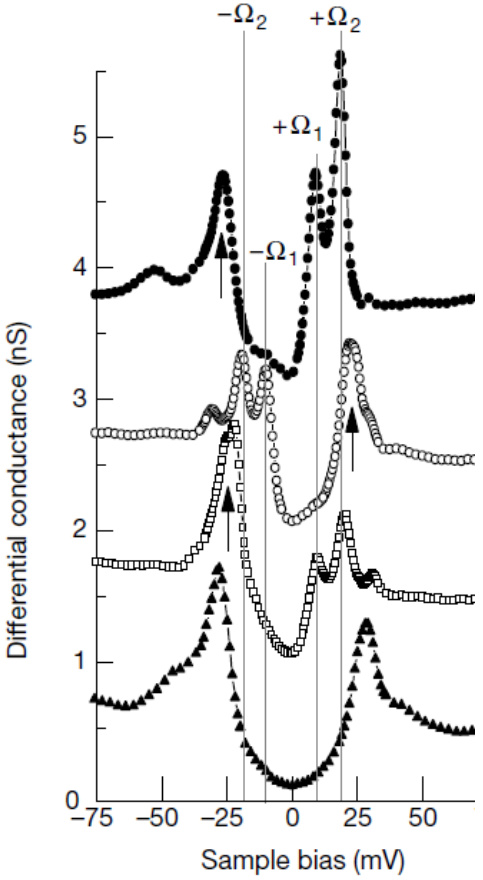
Results: spectra, maps

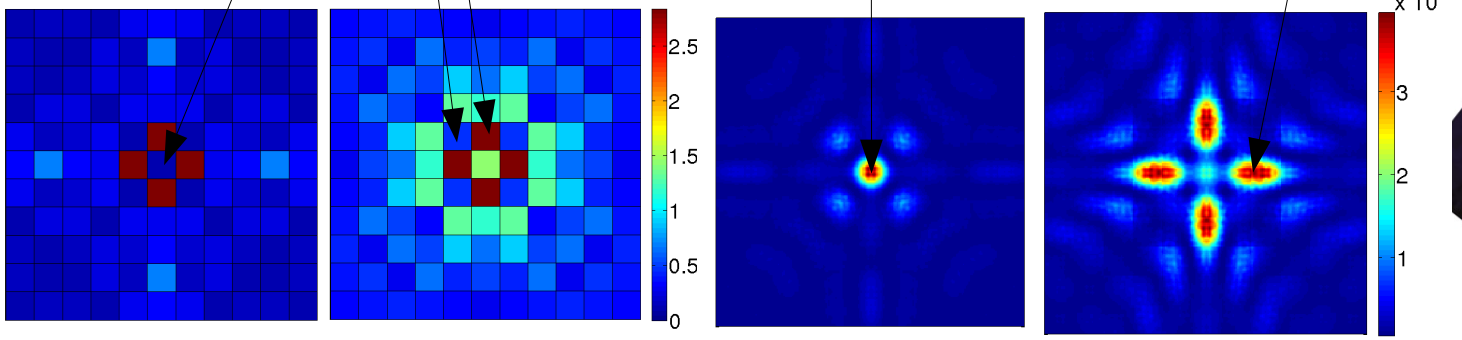


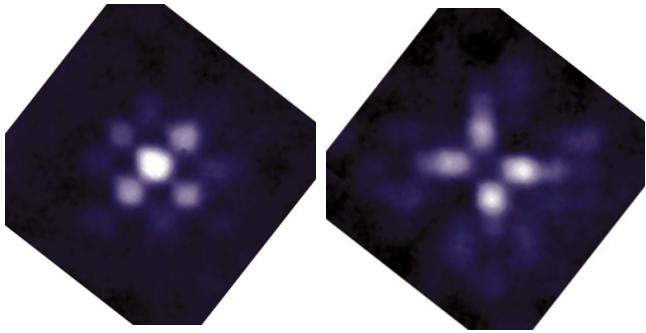












Ω = -2.4 meV

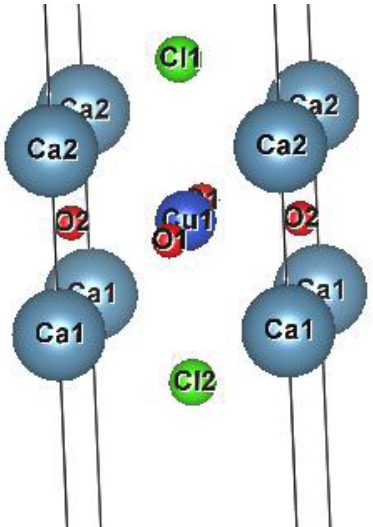
Ω = 2.4 meV

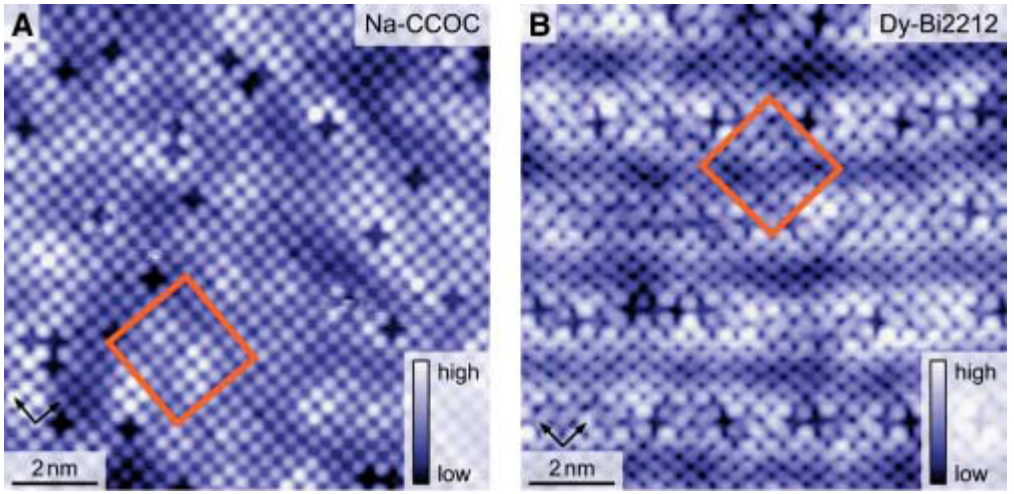
Differences between materials?

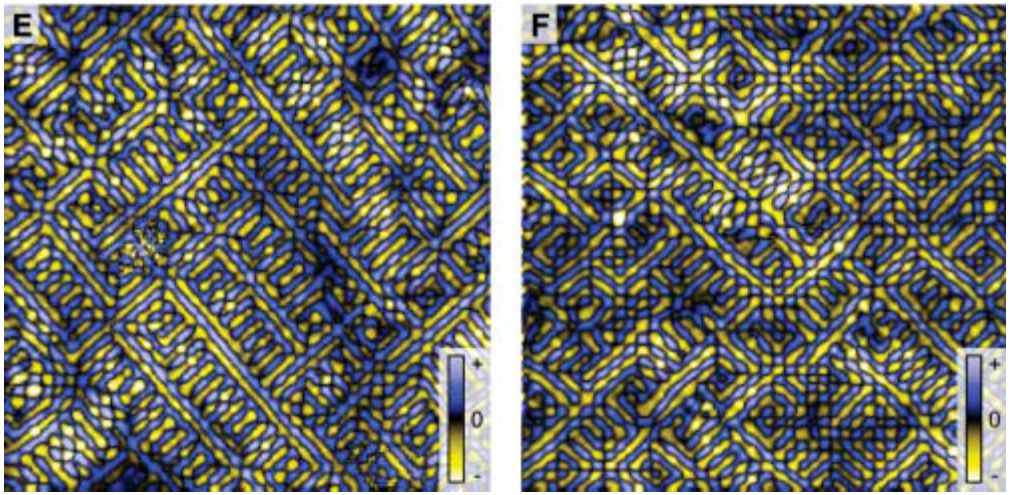
- Different tunnelling layers, same physics

Na-CCOC

Ca-Cl surface

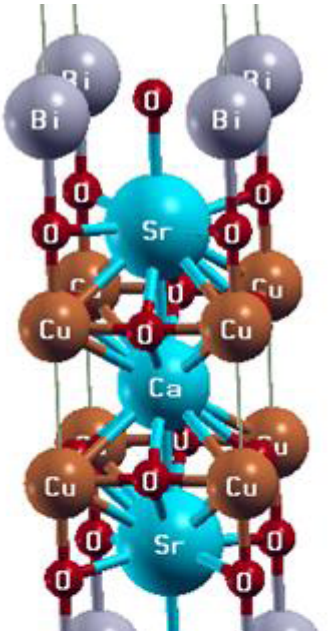




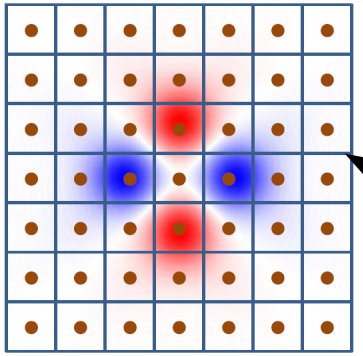


Dy-Bi2212

Bi-O surface
(Sr-O in between)



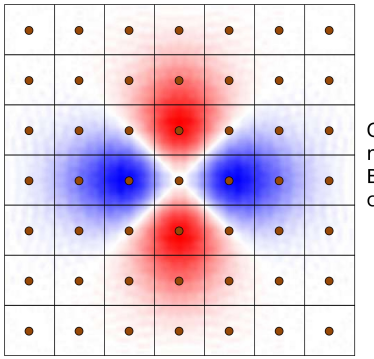
Wannier functions



Na-CCOC

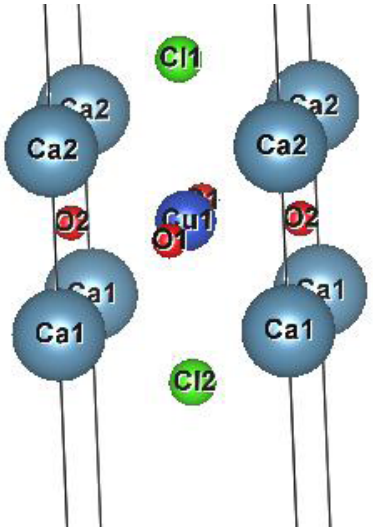
Ca-Cl surface

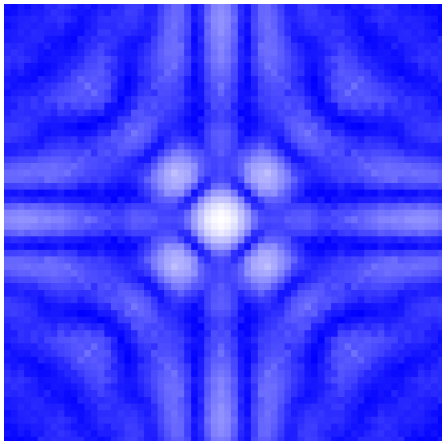
Wavefunctions very similar due to symmetry constraints on downfolding to dx^2-y^2 band in conjunction with crystal symmetry

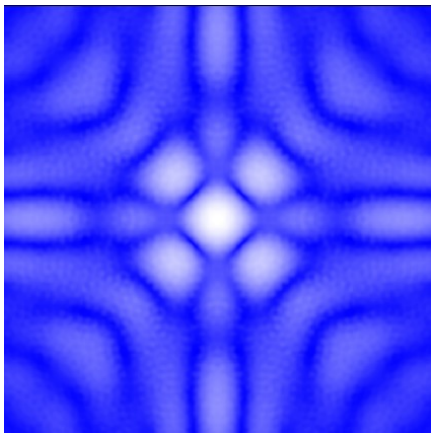


Dy-Bi2212

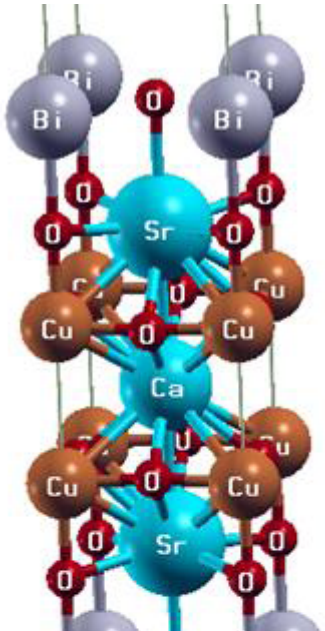
Bi-O surface
(Sr-O in between)







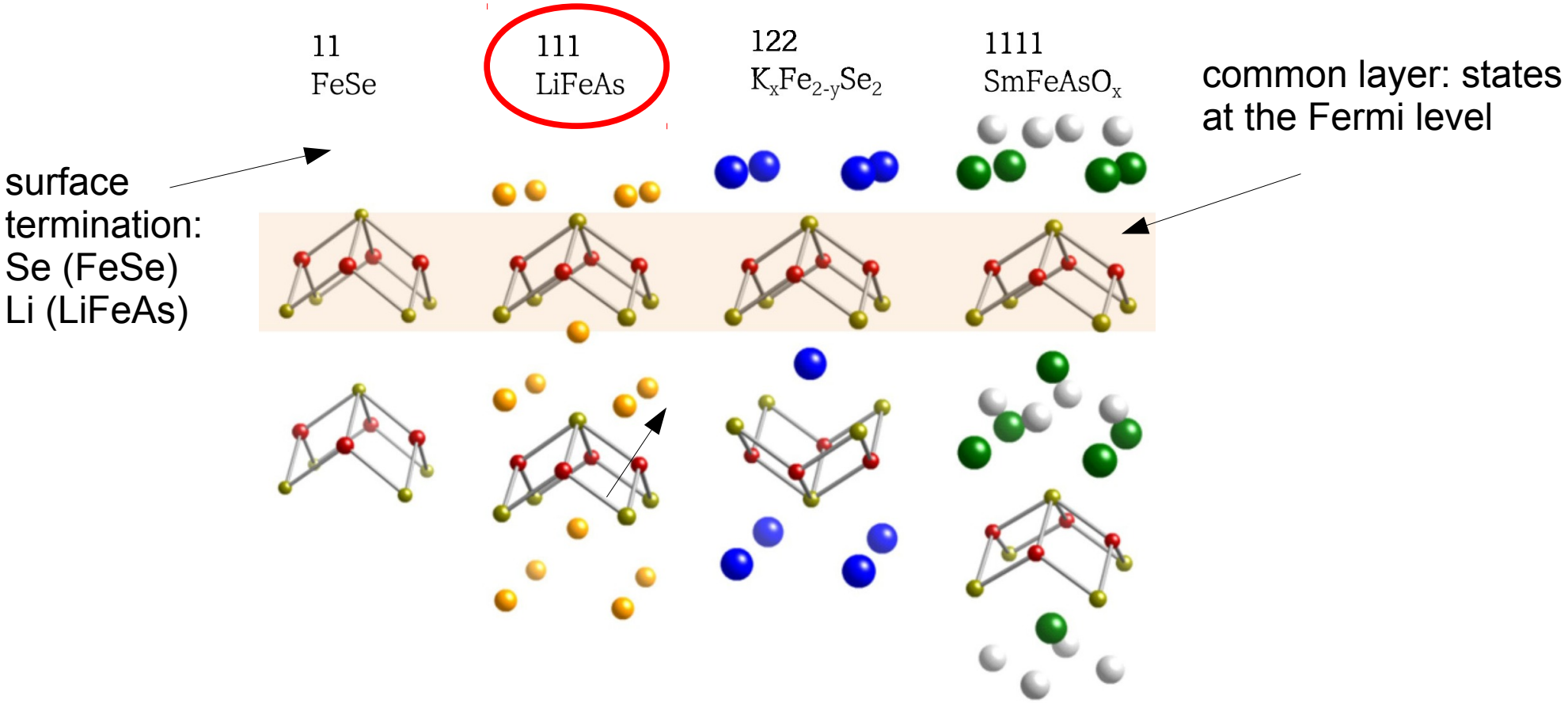
Conductance maps for a strong potential scatterer (in the SC state, d-wave)



Layered superconductors

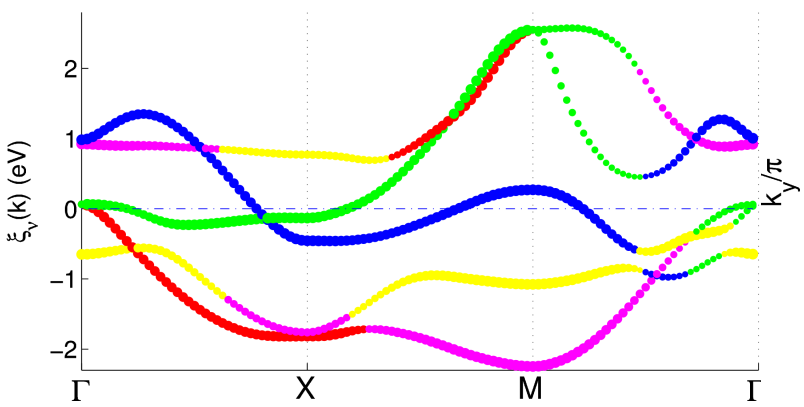
LDOS of sample at given energy at the tip position

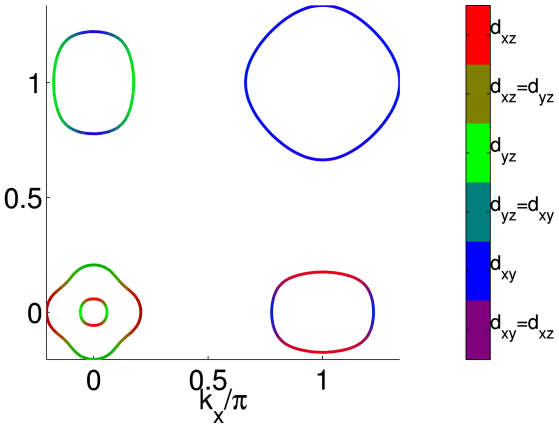
- Iron based superconductors



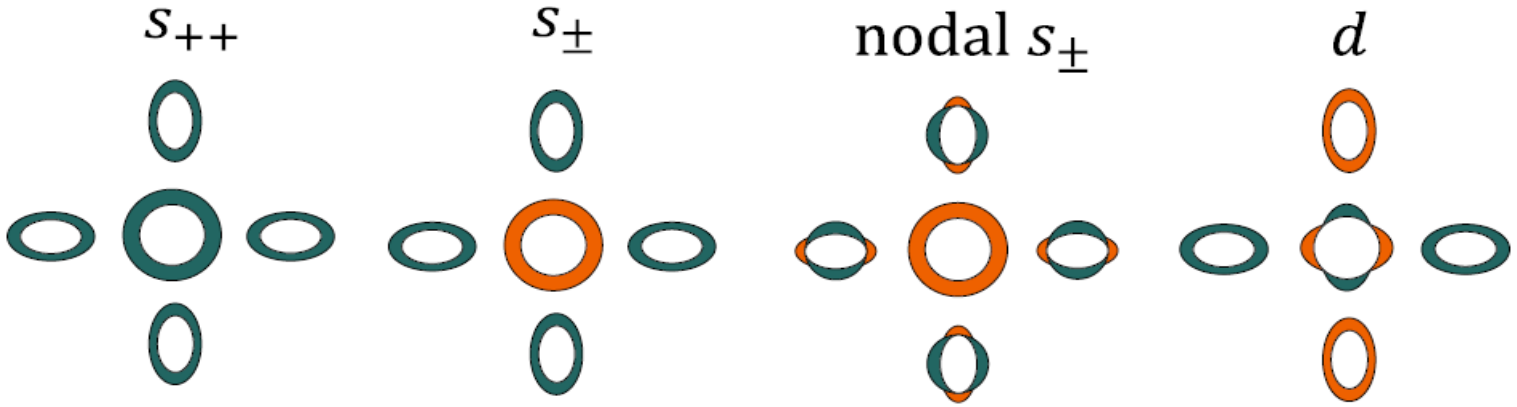
Gap symmetries: FeSC

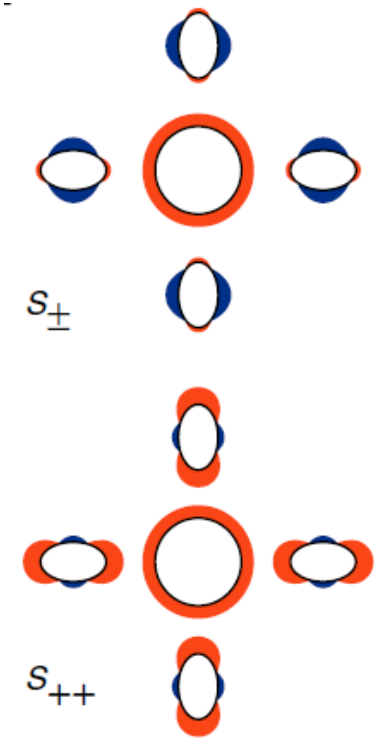
- Fermi surface
  5 band model





- Possible order parameters





P J Hirschfeld, M M Korshunov and I I Mazin, Rep. Prog. Phys. 74 (2011) 124508

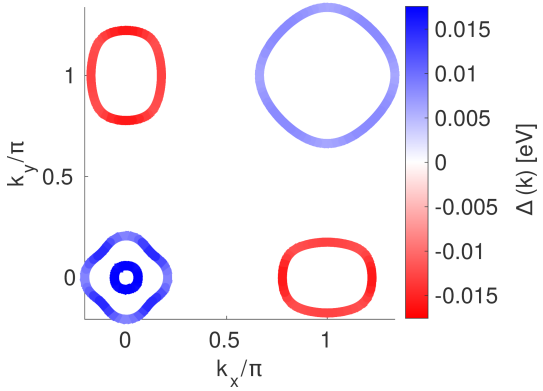
Mizukami, et al. Nat. Commun. 5, 5657 (2014)

LiFeAs: 18K superconductor

- proposed gap structures

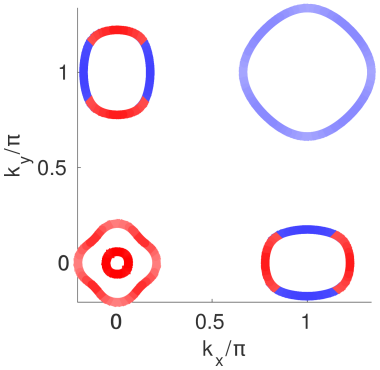
conventional $s_{\pm}$

Y. Wang, A. Kreisel, et al.
Phys. Rev. B 88, 174516 (2013)



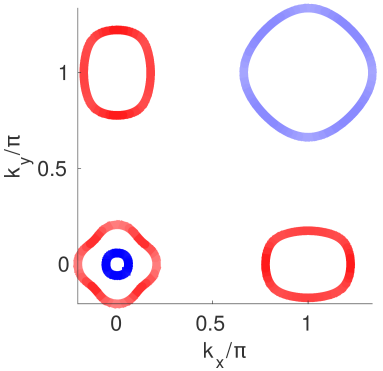
antiphase $s_{\pm}$

Z. P. Yin, K. Haule, G. Kotliar
Nature Physics 10, 845-850 (2014)



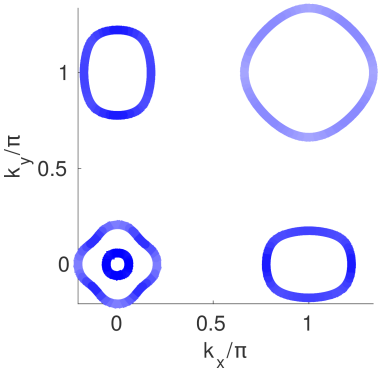
novel $s_{\pm}$

F. Ahn, et al. Phys. Rev. B 89, 144513 (2014)

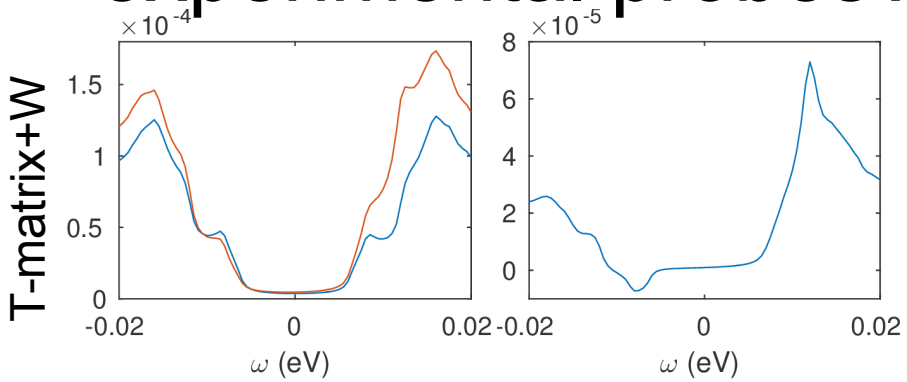


conventional s_{++}

Tetsuro Saito, et al.
Phys. Rev. B 90, 035104 (2014)

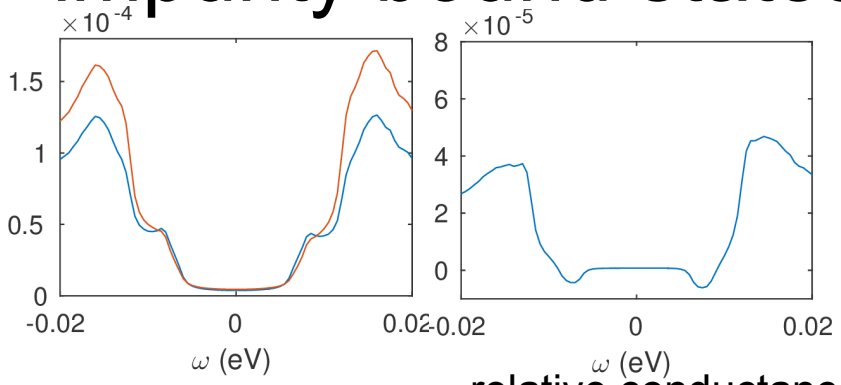


- experimental probes? → impurity bound states



conventional $s_{\pm}$

relative conductance:
peak-dip

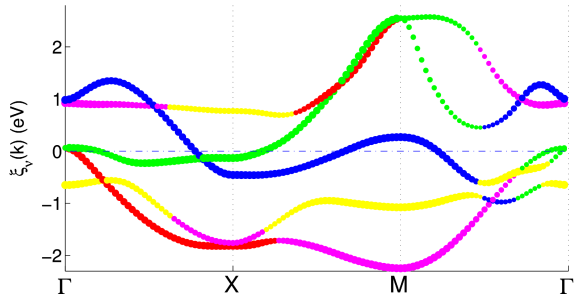


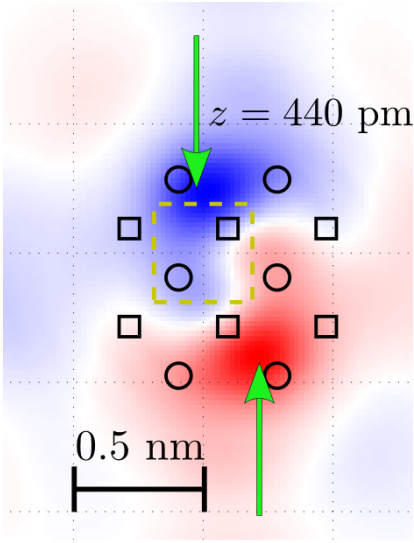
conventional s_{++}

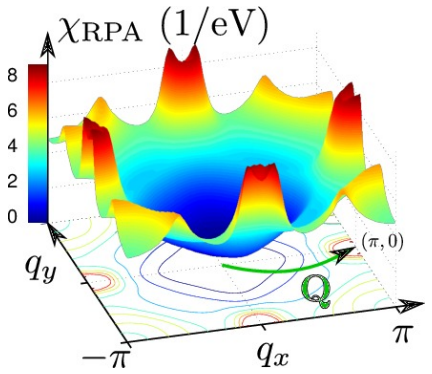
relative conductance:
modification of
normal state DOS

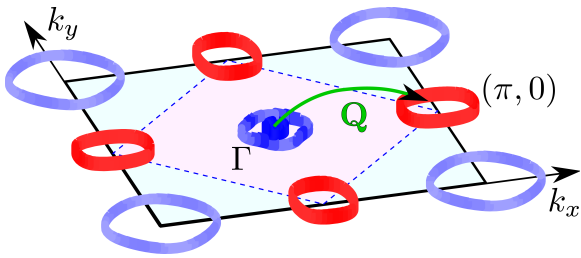
Theory: T-matrix+Wannier

- ab-initio calculation for LiFeAs (surface)
  - tight-binding model (5 band)
  - Wannier functions (including glide plane symmetry)
- superconducting order parameter from spin-fluctuation theory
- ab-initio impurity potentials (Ni, Mn, Co) used in T-matrix calculation









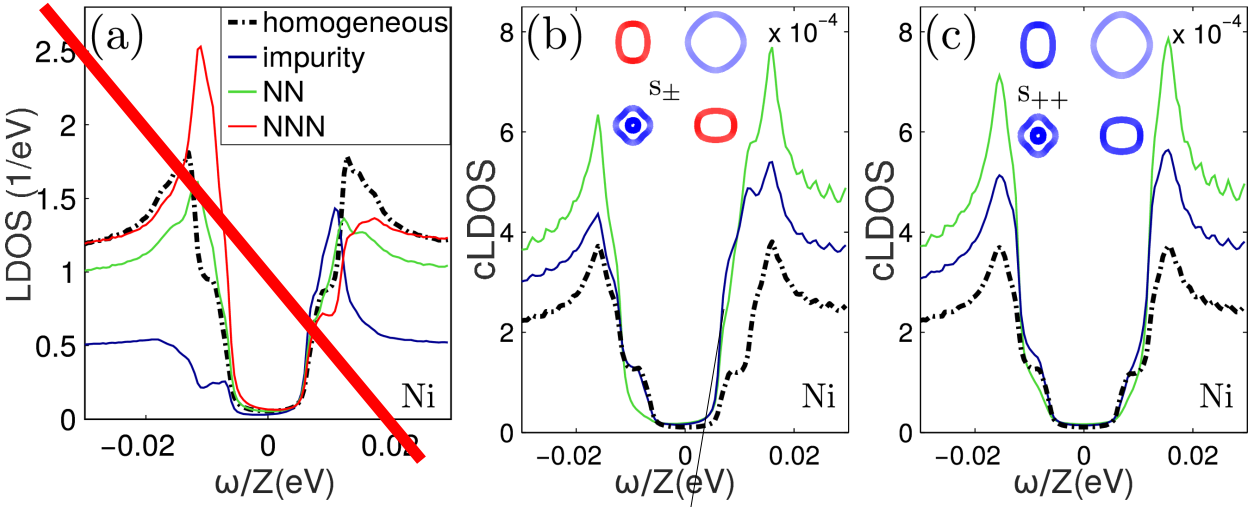
$$\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}_0(\mathbf{r}-\mathbf{r}',\omega) + \hat{G}_0(\mathbf{r},\omega)\hat{T}(\omega)\hat{G}_0(\mathbf{r}',\omega)$$

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

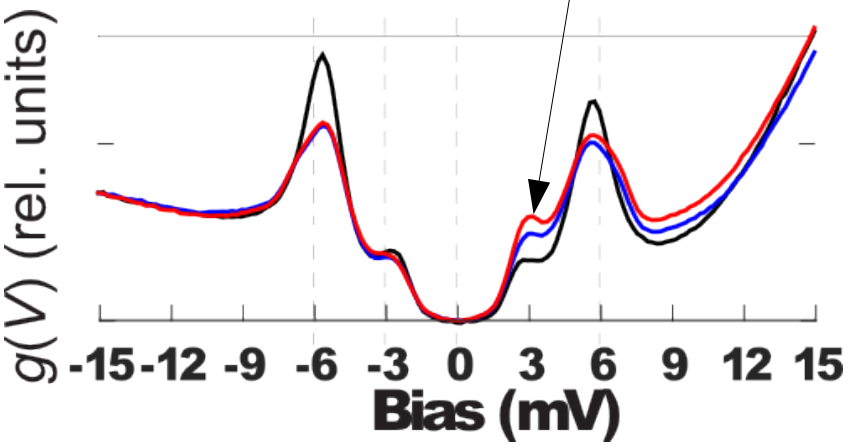
$$\rho(\mathsf{r},\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,G(\mathsf{r},\mathsf{r};\omega)$$

LiFeAs: spectra

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

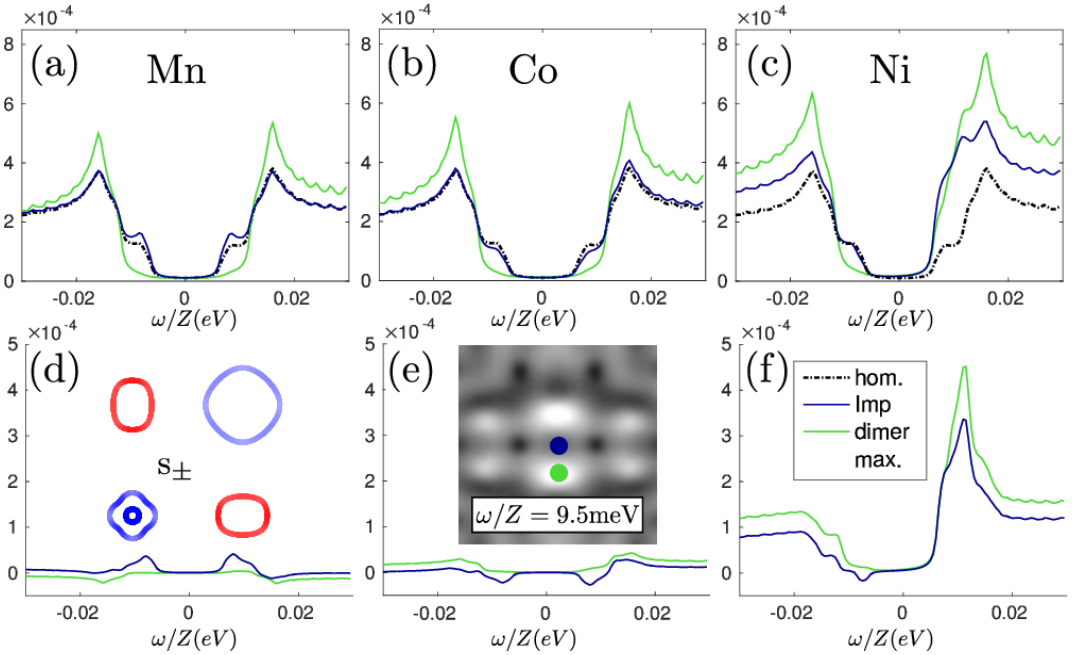


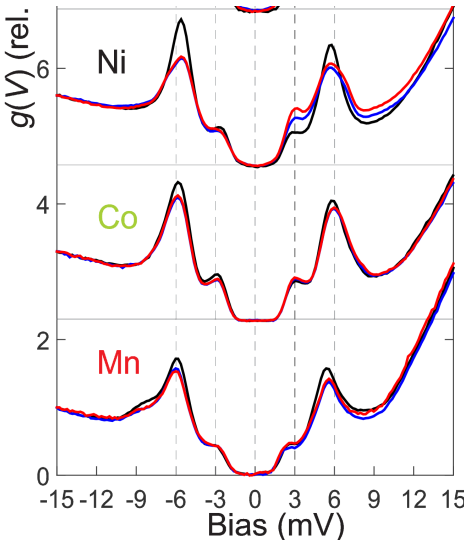
lattice LDOS: strong response at negative bias



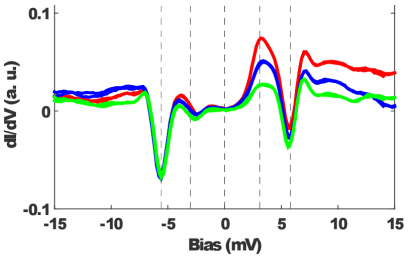
LiFeAs: spectra

- sequence of impurity potentials from ab-initio calculation correct, but overall renormalization downwards required.

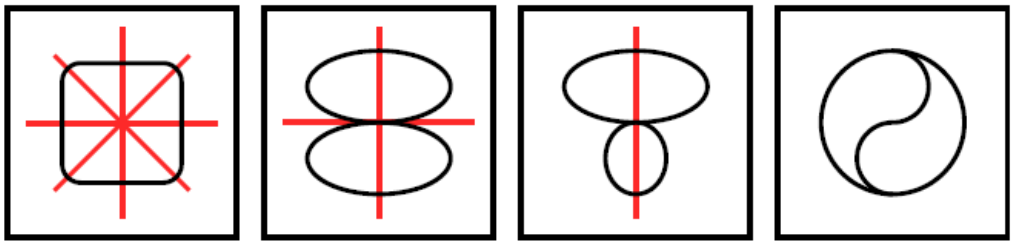




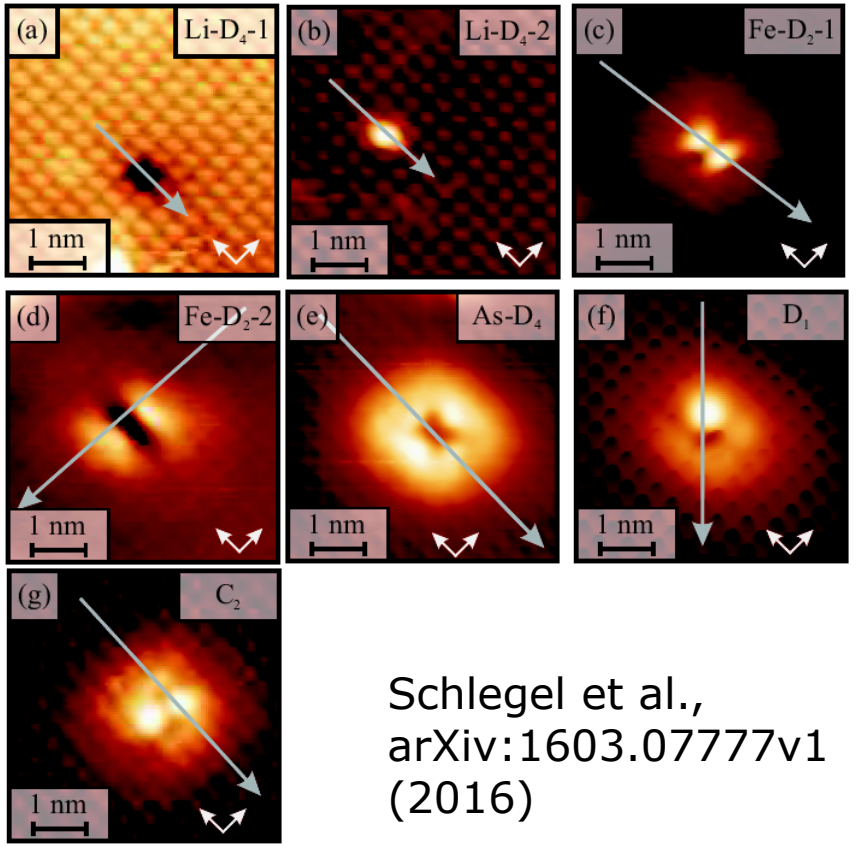
relative spectra
Ni impurity



LiFeAs: other native impurities

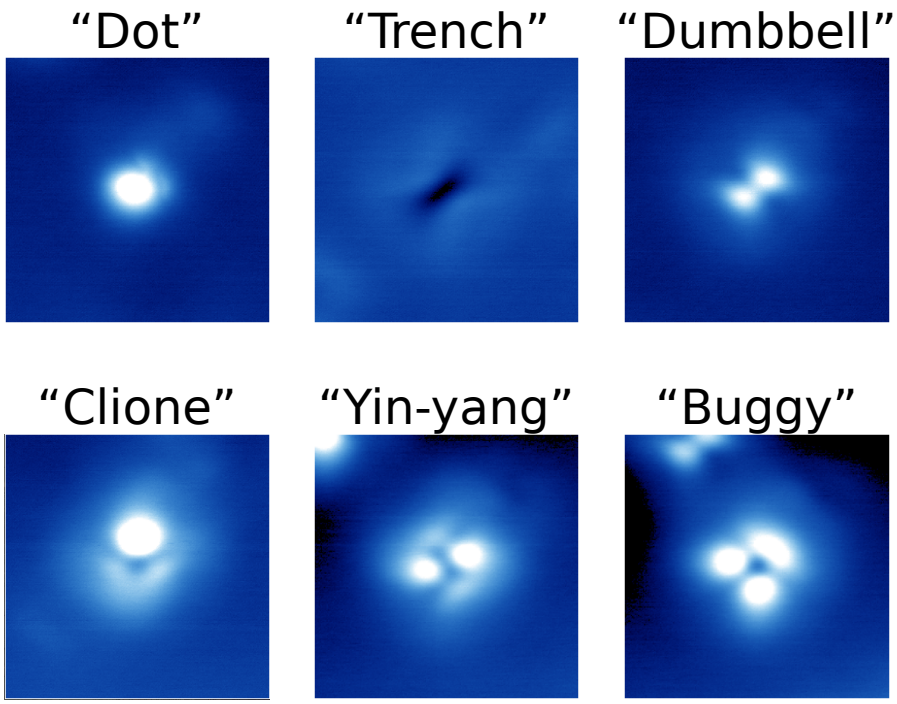


Schönflies classification of impurities



Schlegel et al., arXiv:1603.07777v1 (2016)

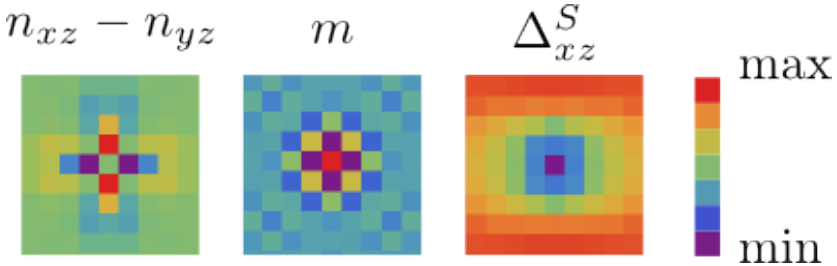
Hanaguri, unpublished (KITP 2011)



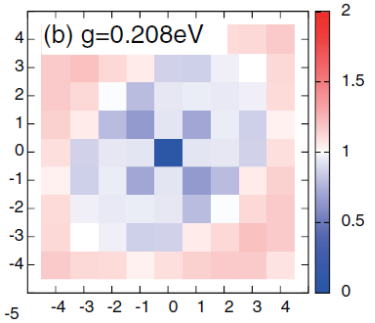
Chiral defects

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

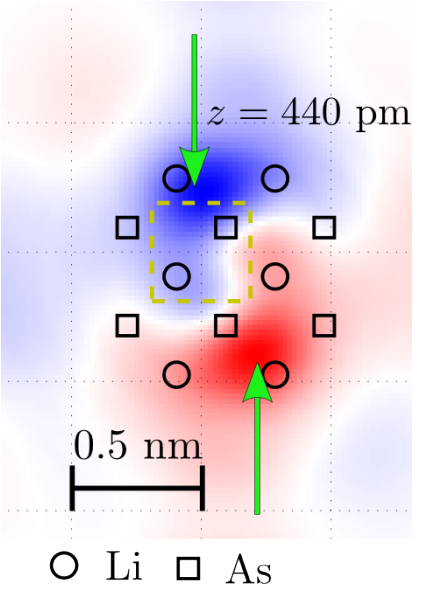
local orbital order
+ Wannier function
→ chiral defect structure



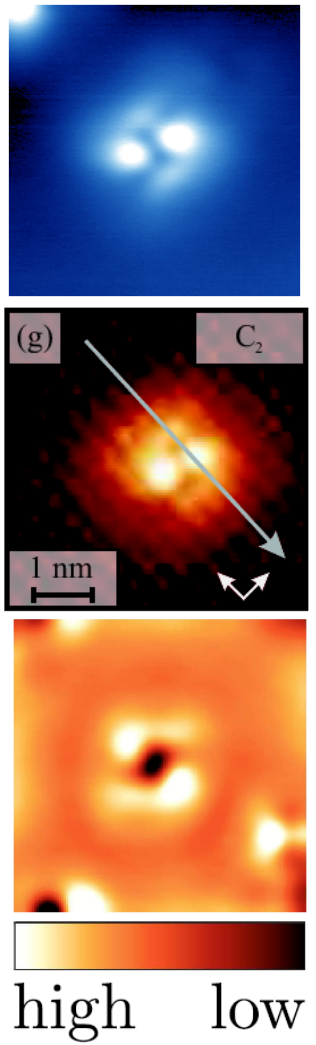
Gastiasoro, Andersen, J. Supercond Nov. Magn., **26**, 2651 (2013)



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

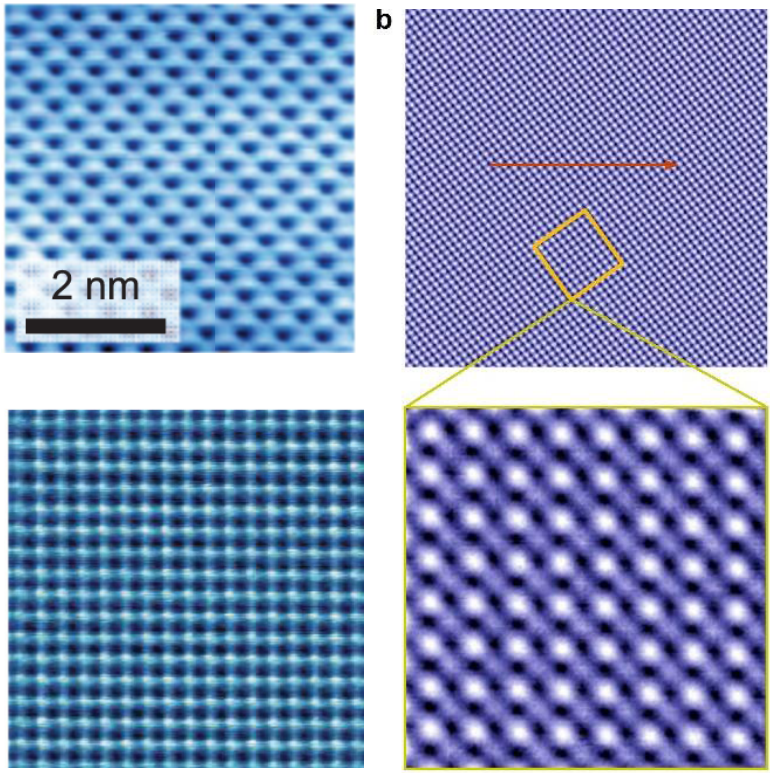


d_xz Wannier function on Fe(2)



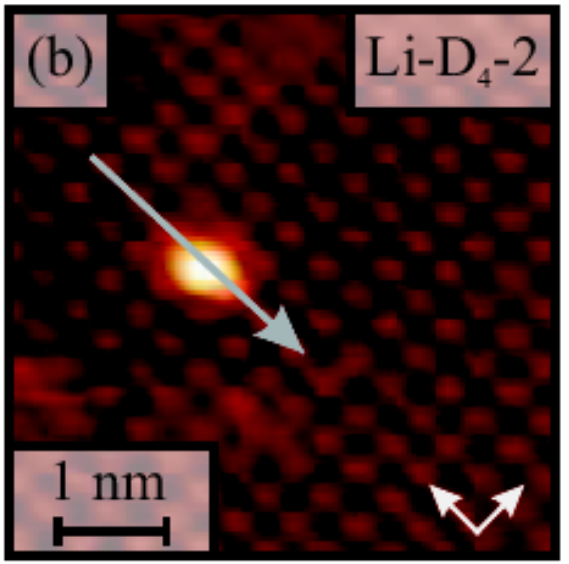
Height and current dependence of topographs

- experiment: 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)

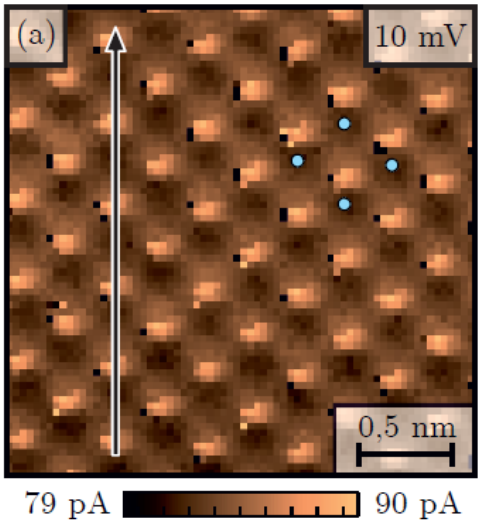
height maxima at Li positions!?
counter-intuitive from chemistry point of view

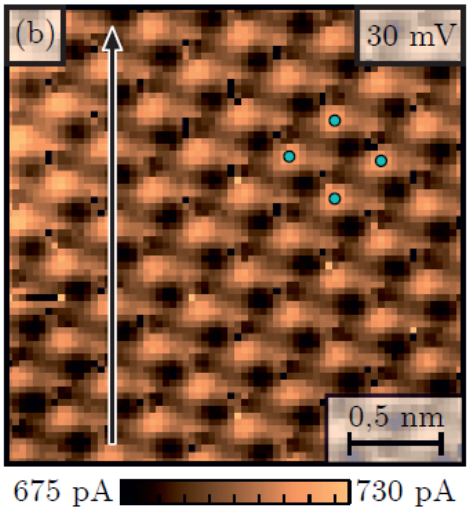


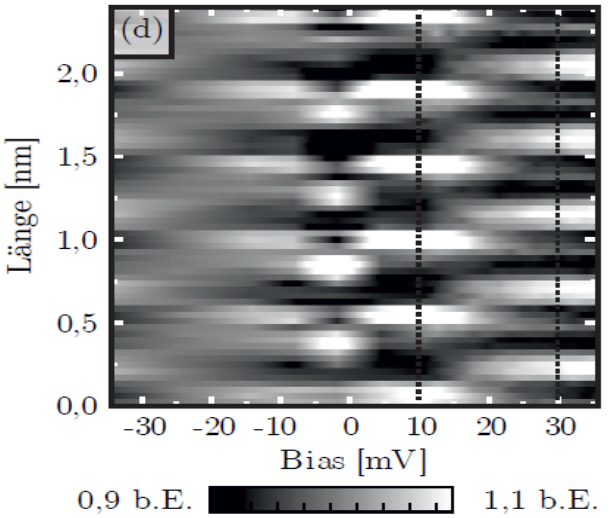
Schlegel et al., arXiv:1603.07777v1 (2016)

Further experimental evidences?

experiment (current maps)

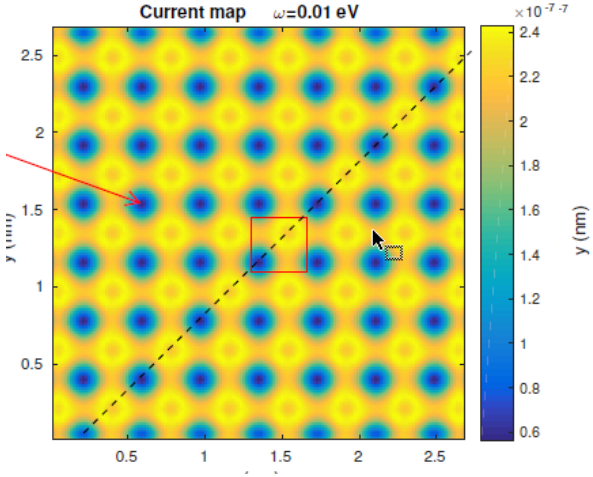


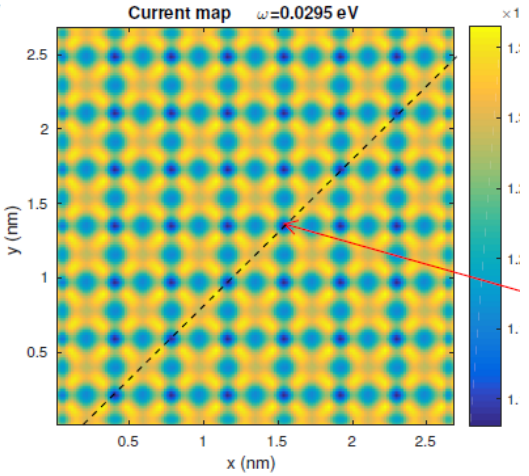


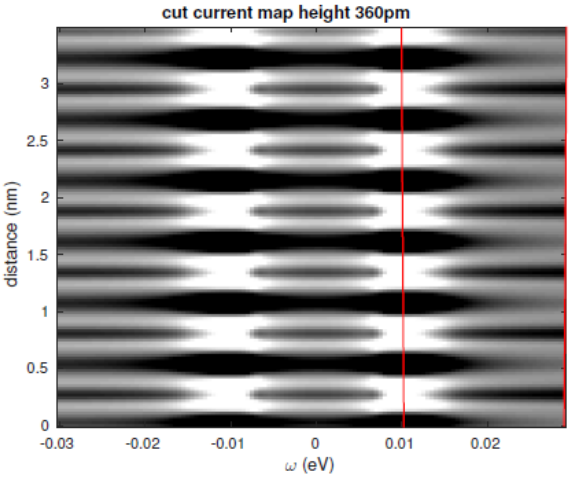


Ronny Schlegel, Dissertation, TU Dresden
(thanks to C. Hess)

theory

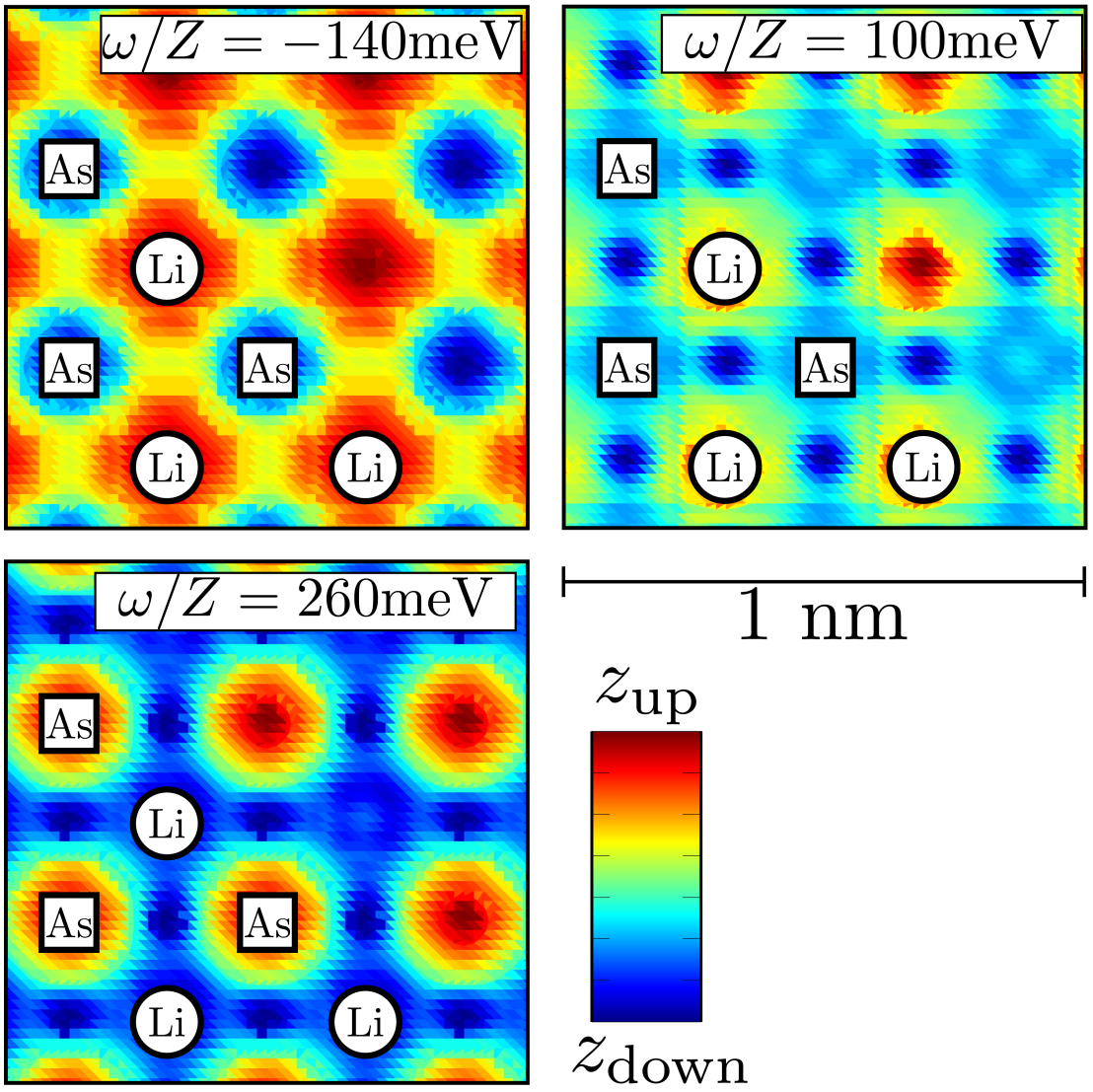






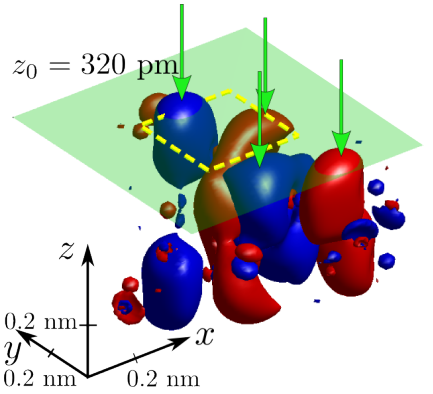
Simulation of topographs

- switching of height maxima as a function of bias voltage

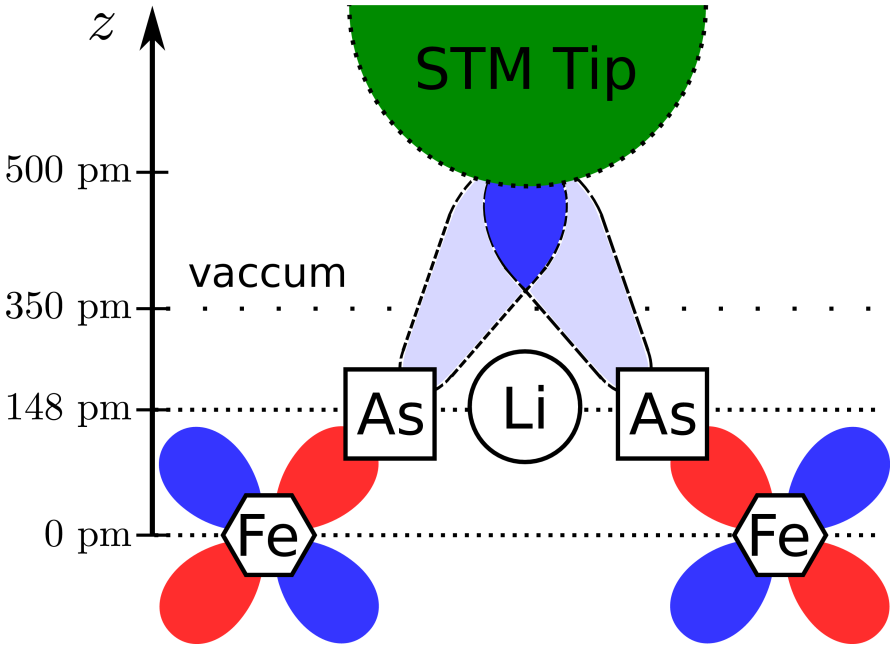


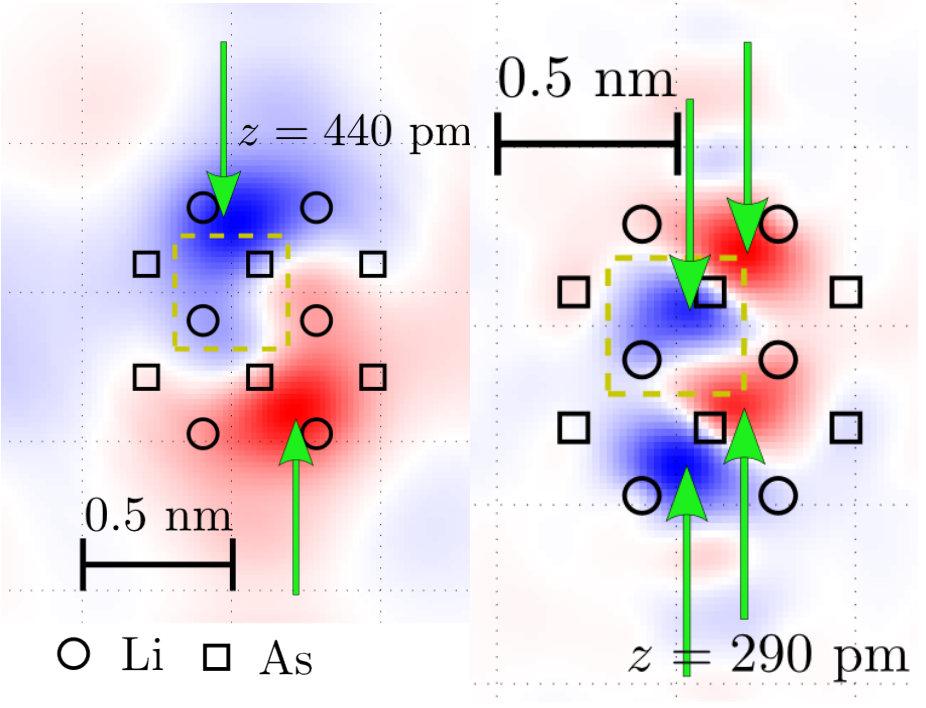
Simulation of topographs

- interplay of interference of wavefunctions and their spatial structure



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



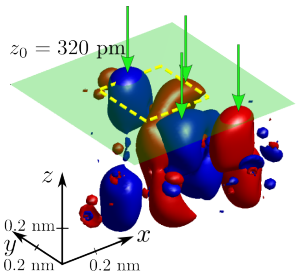


Recapitulation: BdG/T-matrix+W

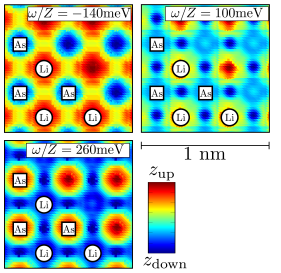
- simple: just a basis transformation of the Green's function

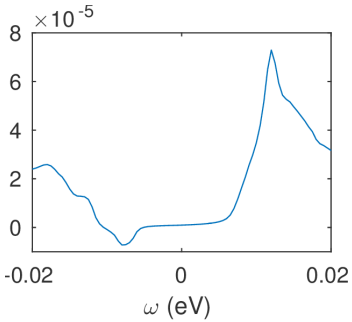
$$G(\mathsf{r}, \mathsf{r}'; \omega) = \sum_{\mathsf{R}, \mathsf{R}'} G(\mathsf{R}, \mathsf{R}'; \omega) w_{\mathsf{R}}(\mathsf{r}) w^*_{\mathsf{R}'}(\mathsf{r}')$$

- powerful tool for calculation of local density of states at the surface (STM tip position) of superconductors

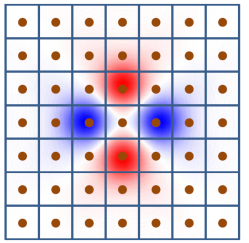


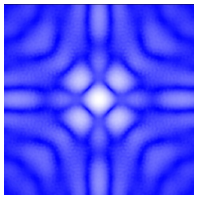
- takes into account atomic scale information and symmetries of the elementary cell and the contained atoms

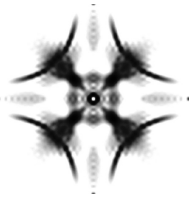




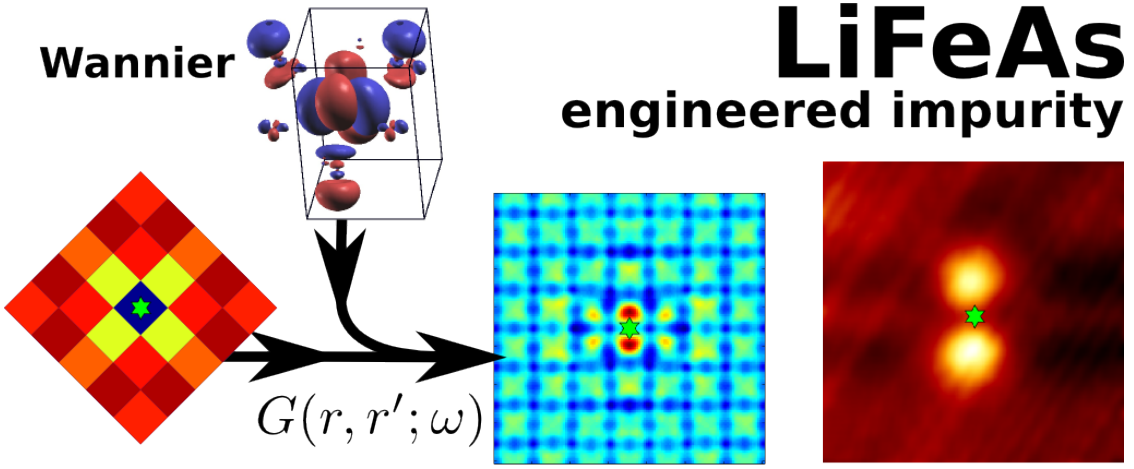
- shown to work
  - LiFeAs: metal ion impurities
    Shun Chi, (...), A. Kreisel, et al. arXiv:1607.03192
  - BiSrCaCuO: Zn impurity, QPI
    Kreisel *et al.* PRL **114**, 217002 (2015)





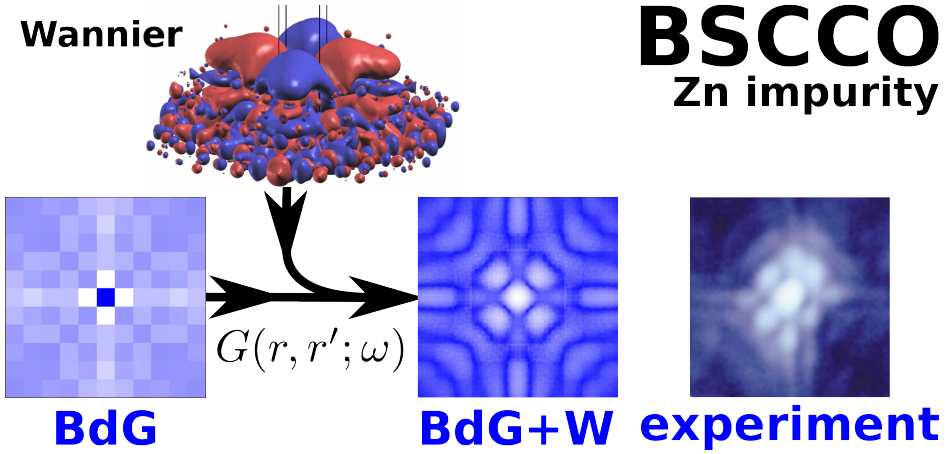


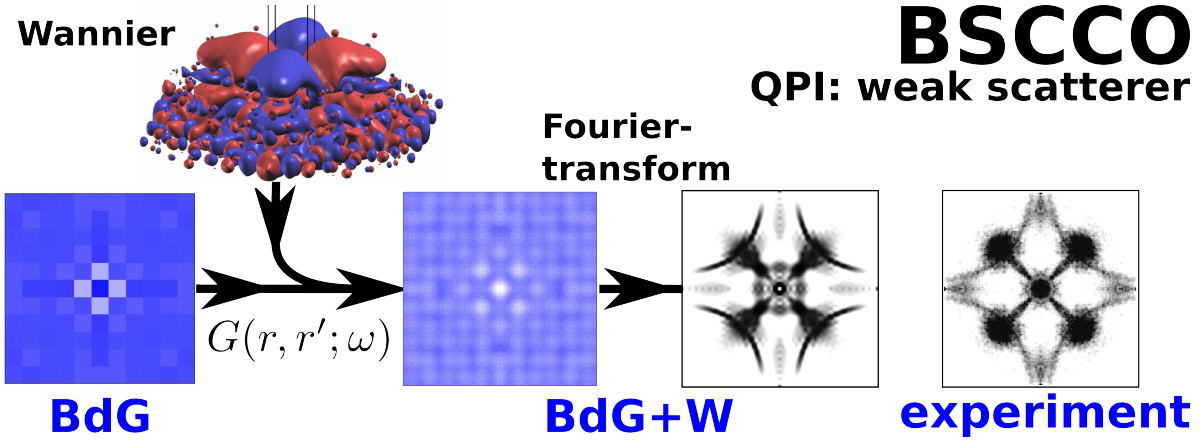
Summary



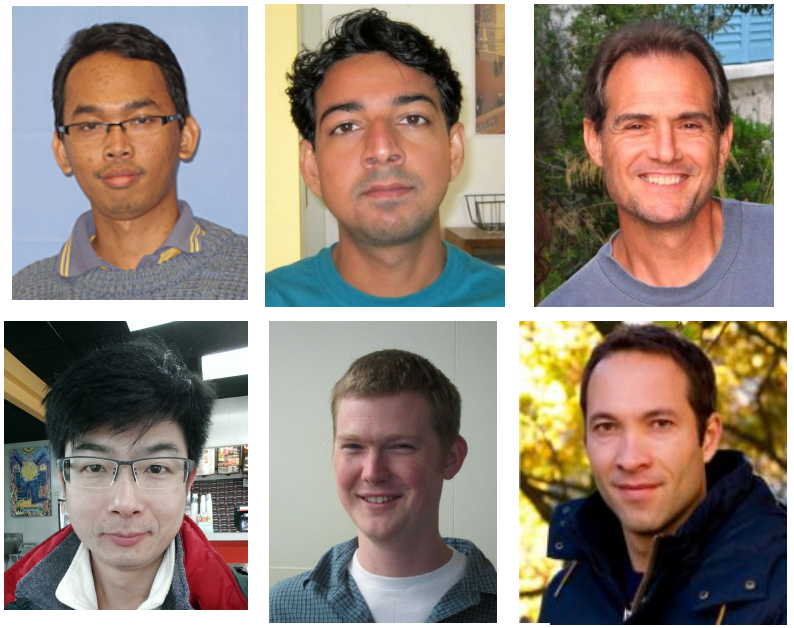
Kreisel *et al.*
PRL **114**, 217002 (2015)

arXiv:1607.03192





Acknowledgements

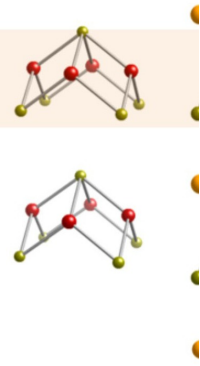


University of St Andrews

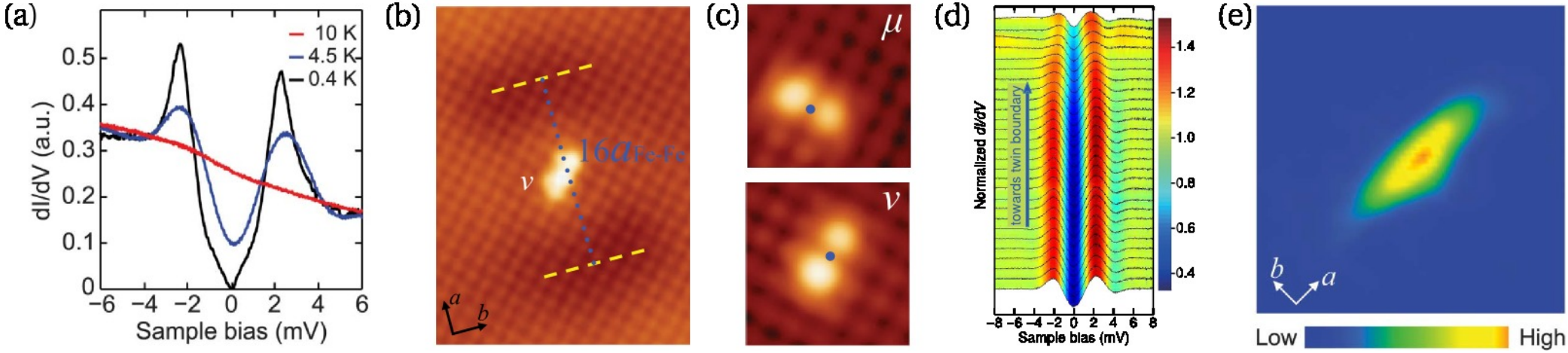
THE UNIVERSITY OF BRITISH COLUMBIA

FeSe: simplest crystal structure

11
FeSe



- Tc 8K, under pressure ~40K — Medvedev, et al. Nat. Mater. 8, 630 (2009)
- Tc 100K (single layer) — Ge et al. Nat. Mater. 14, 285 (2015)
- nematic phase
  no magnetism — Baek, et al. Nat. Mat. 14, 210 (2015)
- consequences: nodal gapstructure, anisotropy



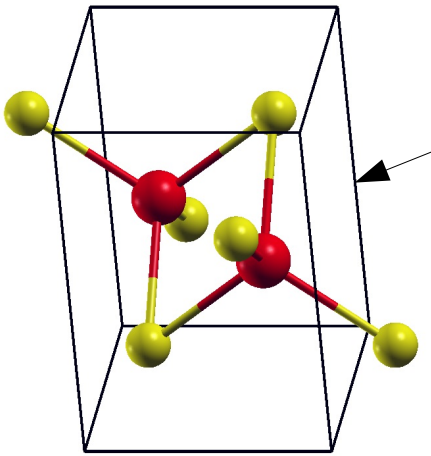
Song et al. PRL 109, 137004 (2012)

Song et al. Science 332, 1410 (2011)

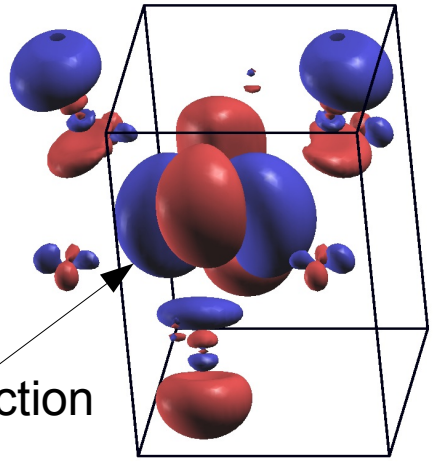
BdG+Wannier method

- first principles calculation
  - band structure
  - Wannier functions wavefunctions in real space

$$H_0 = \sum_{\mathsf{R}\,\mathsf{R}',\sigma} t_{\mathsf{R}\,\mathsf{R}'} c^\dagger_{\mathsf{R}\,\sigma} c_{\mathsf{R}'\sigma} - \mu_0 \sum_{\mathsf{R},\sigma} c^\dagger_{\mathsf{R}\,\sigma} c_{\mathsf{R}\,\sigma}$$



elementary cell of FeSe



Wannier function with phases centered at Fe(I)

Fe(I)-d_{xy}

- continuum Green function

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

continuum position

nonlocal contributions

lattice Green function

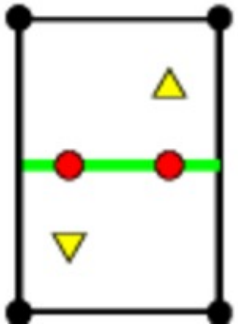
local density of states (LDOS)

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

FeSe: BdG+W Results

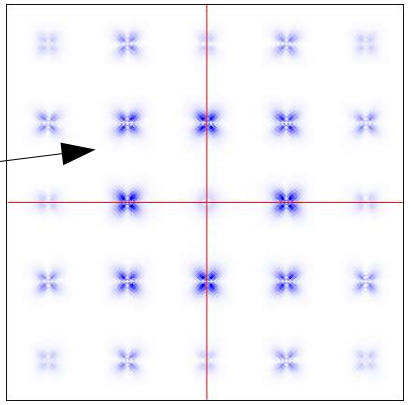
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

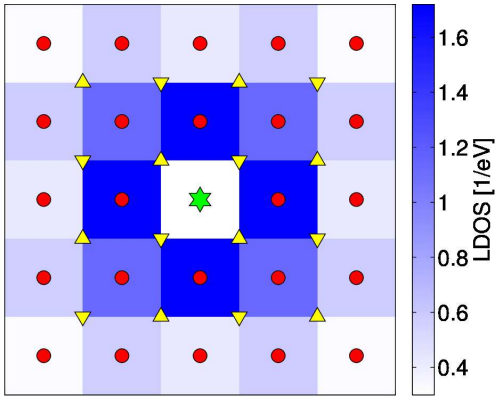
- continuum density of states
  - at Fe plane



C4 symmetry!

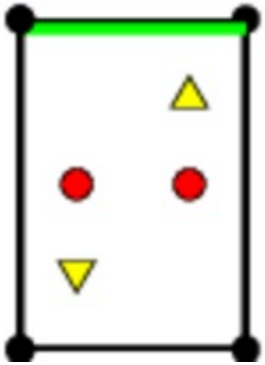
2 meV

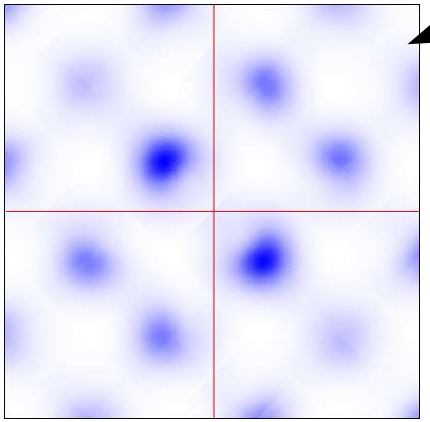


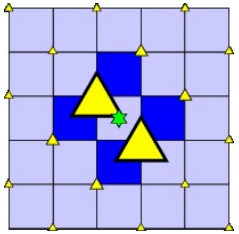


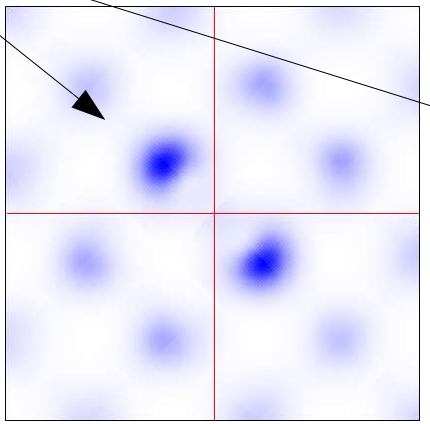
  - at STM tip position

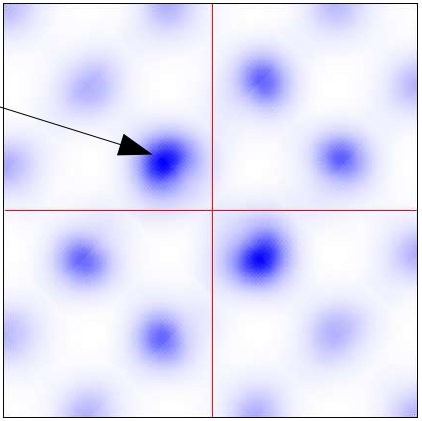
C2 symmetry!











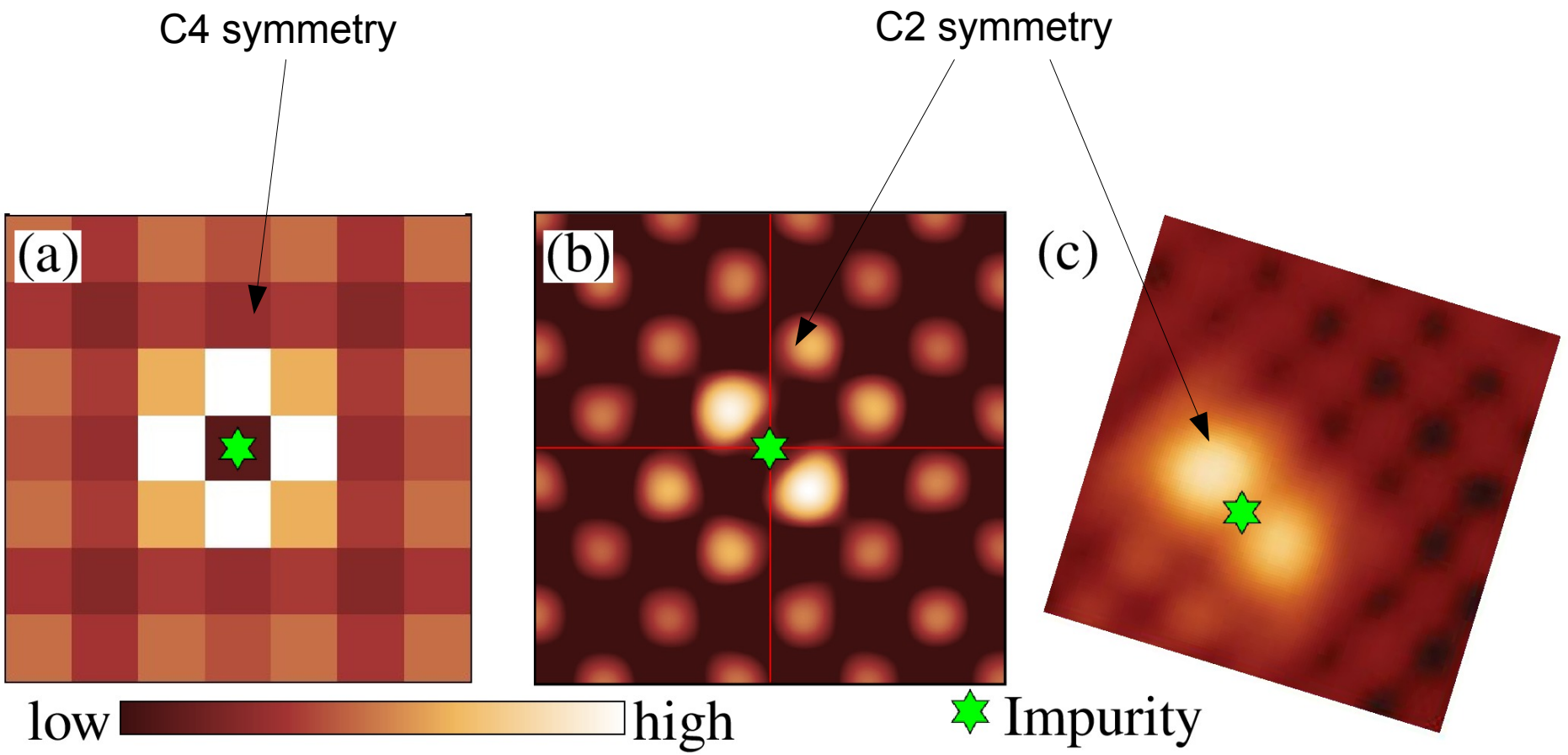
-2 meV

+2 meV

+30 meV

FeSe: Comparison to experiment

STM topography on (bulk) FeSe with Fe-centered impurity



BdG

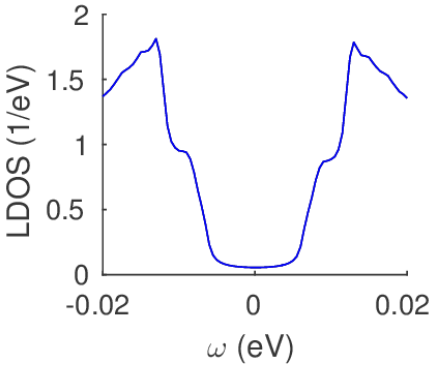
BdG+W

experiment

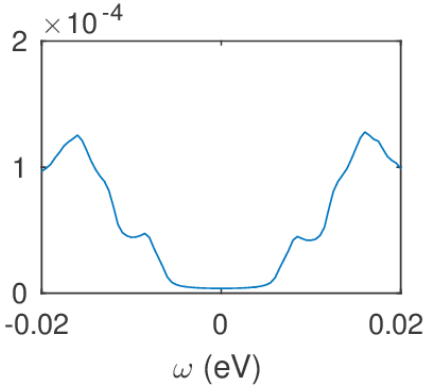
Can-Li Song, *et al.* PRL **109**, 137004 (2012)

LiFeAs: spectra

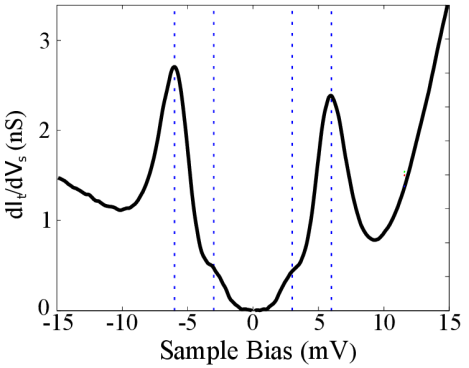
T-matrix



T-matrix+Wannier (T+W)

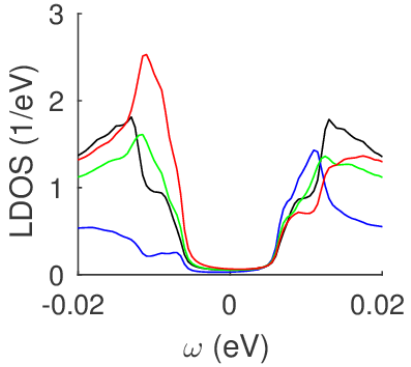


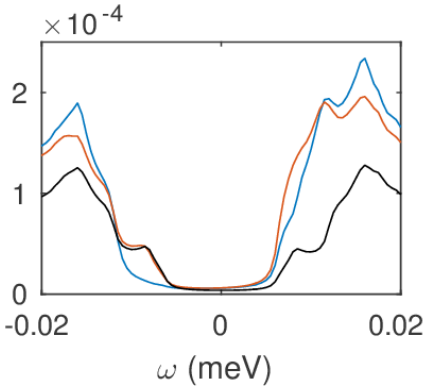
experiment



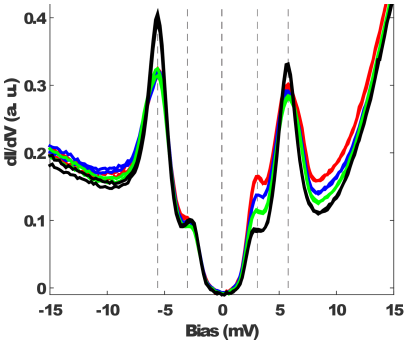
Chun Chi
PhD thesis

Ni impurity potential (*ab initio*)



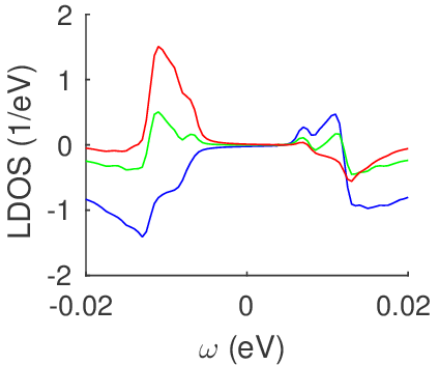


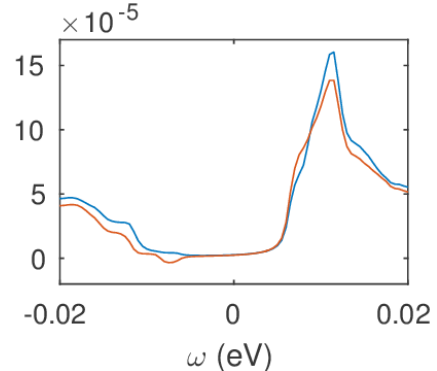
engineered Ni impurity

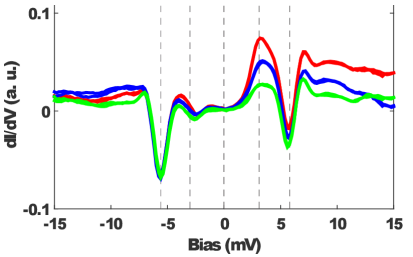


Chun Chi
et al. (in
preparation)

relative spectra



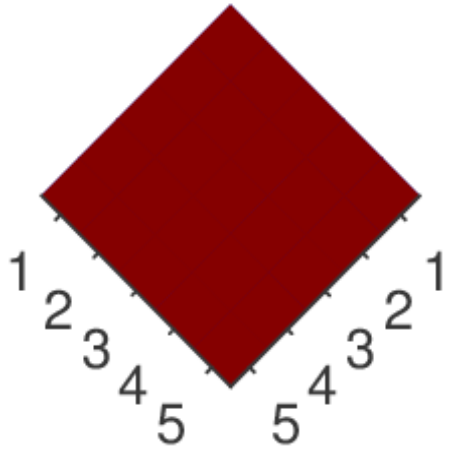




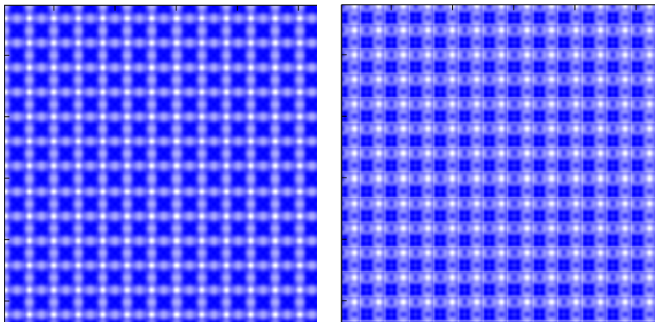
LiFeAs: spatial conductance

T-matrix

homogeneous



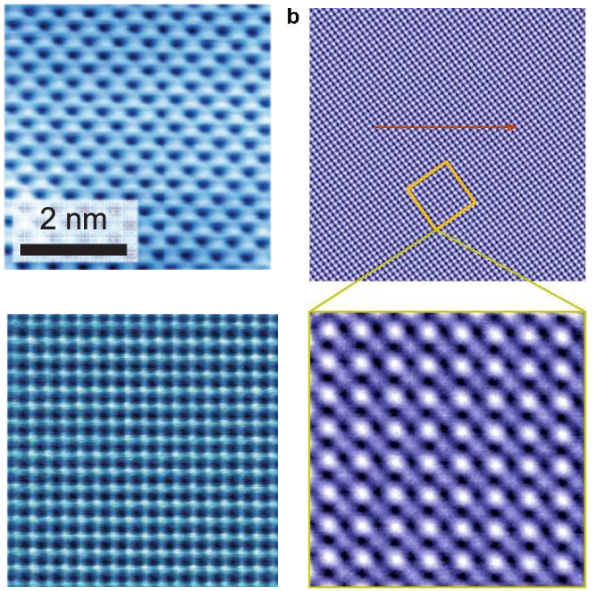
T-matrix+Wannier (T+W)



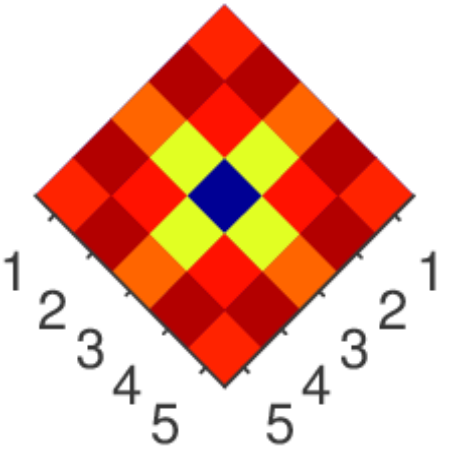
variation of tip heigh:

As lattice Li lattice

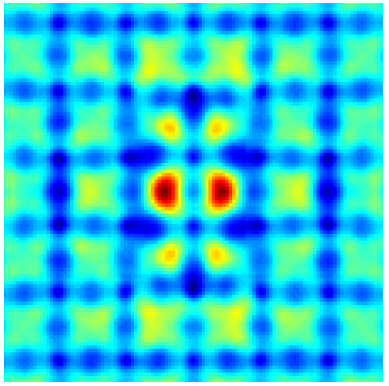
experiment (Li ↔ As lattice ?)



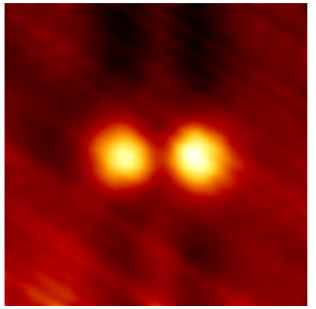
one pixel per Fe atom!



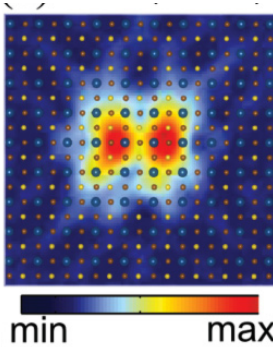
Ni impurity:
C2 symmetric impurity state



engineered
Ni defect



Fe centered
defect



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)