Theory of STM on Unconventional Superconductors

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The Foundation for The Gator Nation

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)
P. Choubey, *et al.*. Phys. Rev. B **96**, 174523 (2017)

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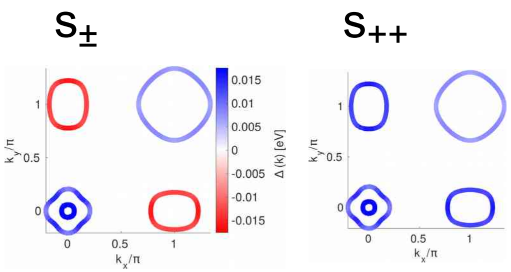
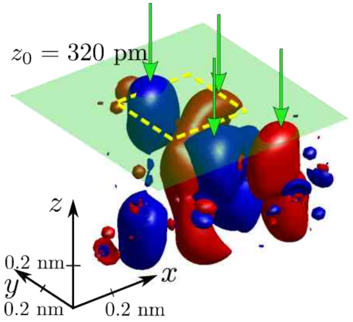
Outline

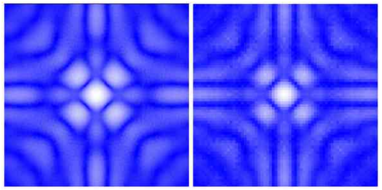
- Motivation
  - STM: impurities as probe for electronic structure, order parameter and more
  - layered superconductors, complications



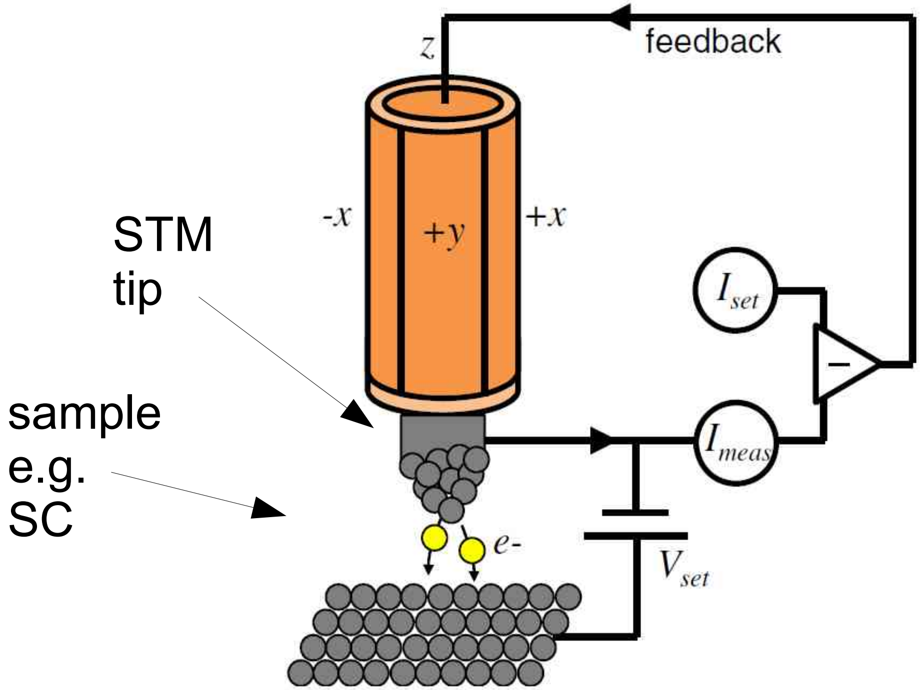
- Theoretical methods to investigate impurity physics in superconductors
  - using wavefunction information in layered superconductors: Wannier method
  - Applications
    - LiFeAs (multiband, s-wave)
    - Cuprates: $Bi_2Sr_2CaCu_2O_8$, $Ca_2CuO_2Cl_2$



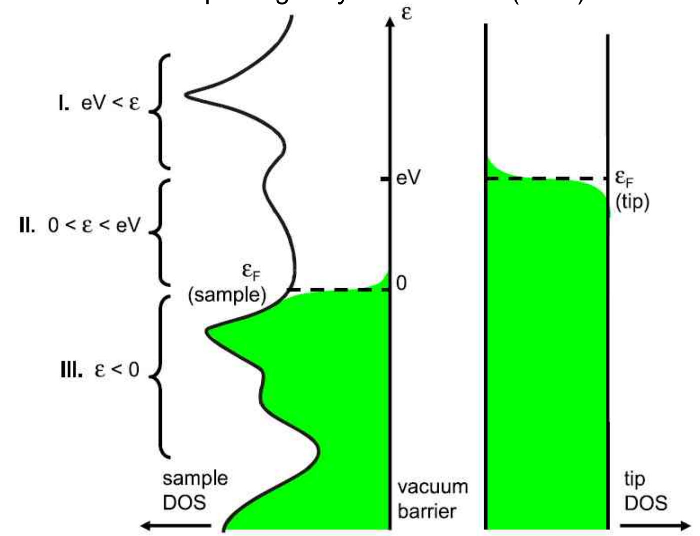
- Inelastic tunneling



Scanning tunneling microscopy



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

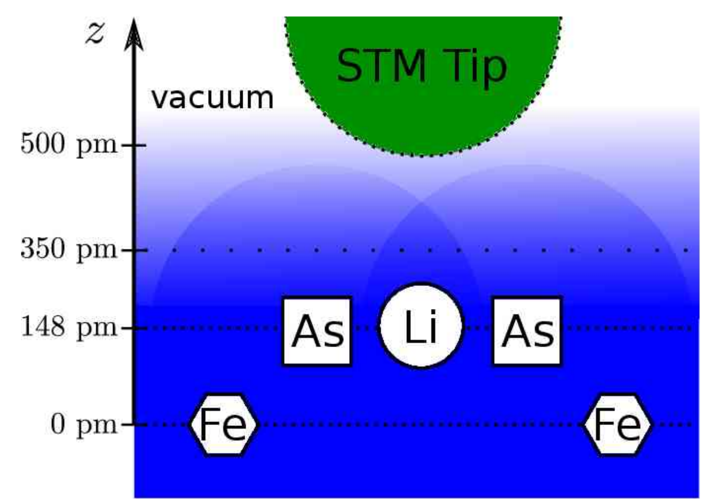


Tunneling current:

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

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

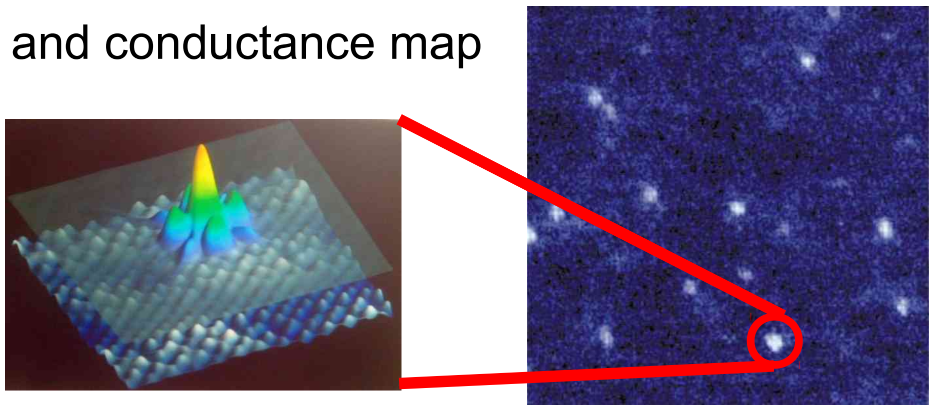
J. Tersoff and D. R. Hamann, PRB **31**, 805 (1985)



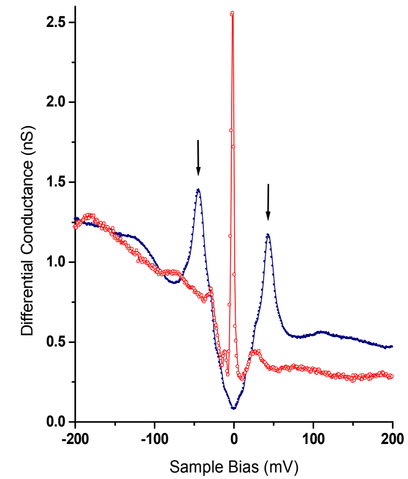
STM: examples

- Cuprates: Zn impurity in BSCCO

spectra and conductance map

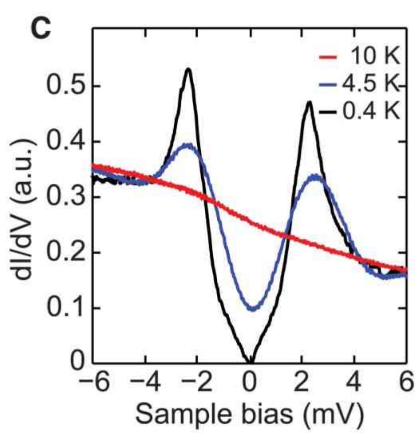


Pan et al., Nature **403**, 746 (2000)

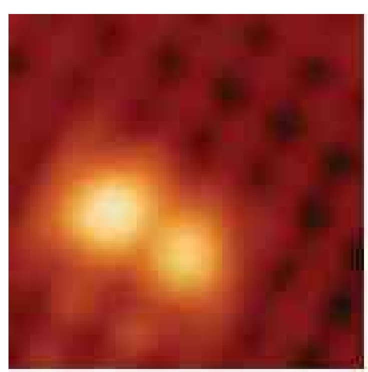


- Fe-SC

FeSe: topograph of Fe centered impurity

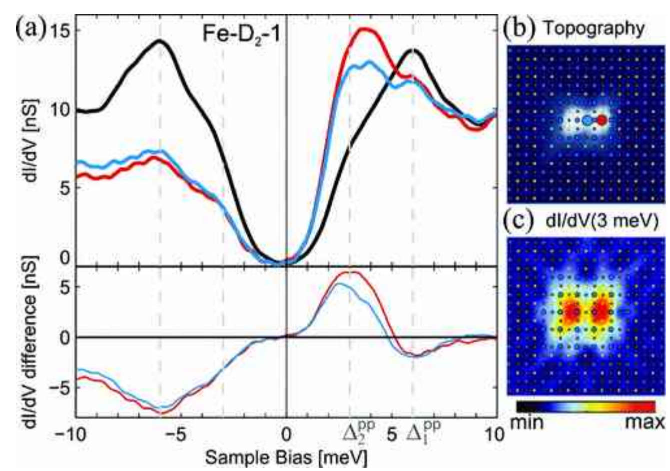


Song et al., Science **332**, 1410 (2011)



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

LiFeAs: Fe centered impurity



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

Layered superconductors

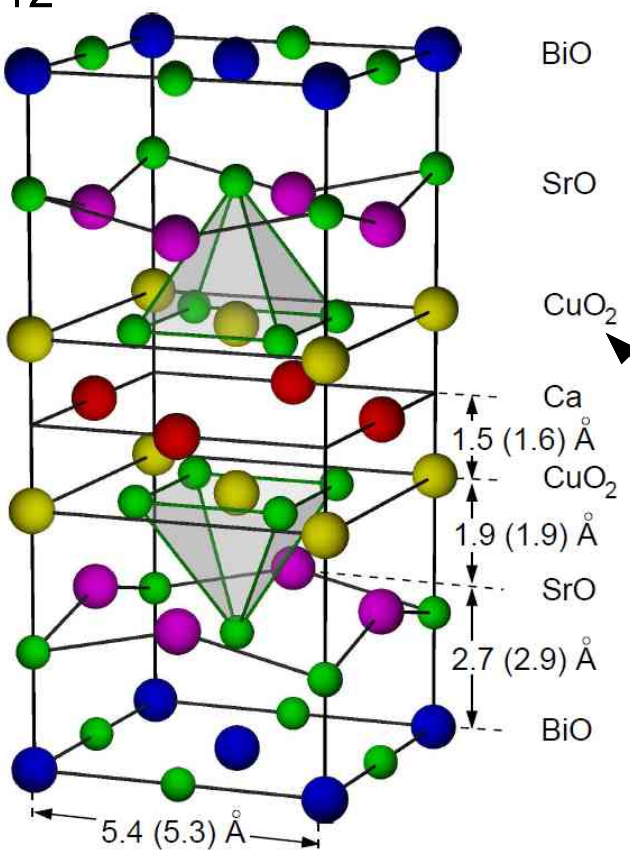
- 2 examples: surface atoms ≠ superconducting layer

Cuprates

Iron based superconductors

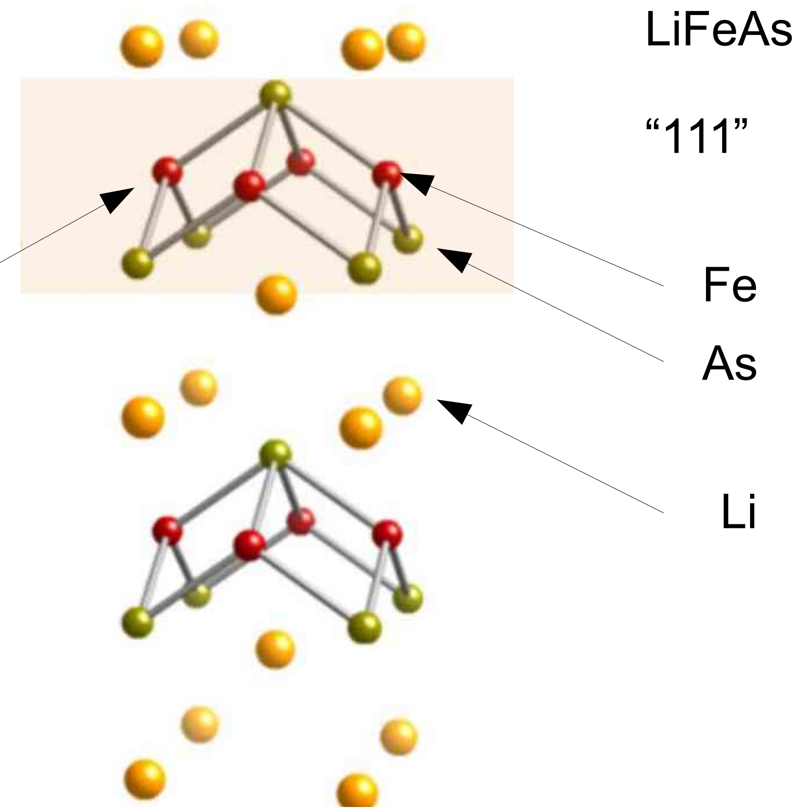
surface: BiO

Bi-2212



states at the Fermi level
Cu-plane
Fe-plane

surface: Li, As?



Theoretical approaches: Cuprates

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

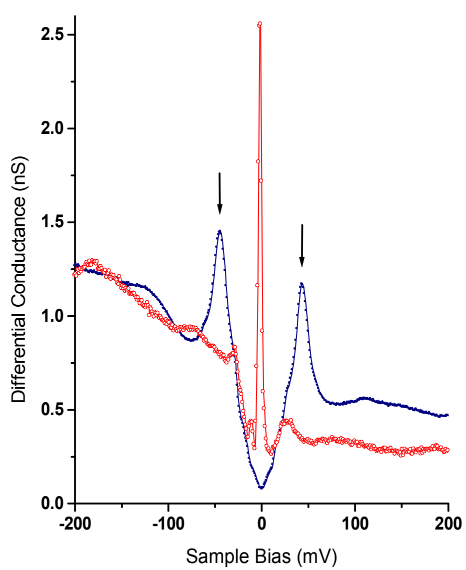
$$\Omega \equiv \Omega' + i\Omega'' = \Delta_0 \frac{\pi c/2}{\ln(8/\pi c)} \left[1 + \frac{i\pi}{2} \frac{1}{\ln(8/\pi c)} \right]$$

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

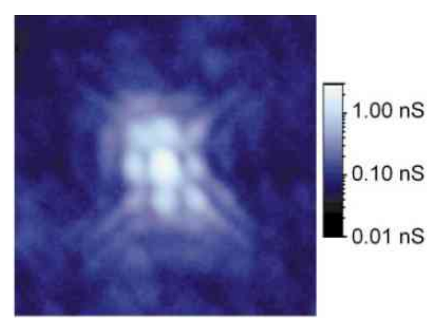
A. V. Balatsky, M. I. Salkola, and A. Rosengren Phys. Rev. B **51**, 15547 (1995)

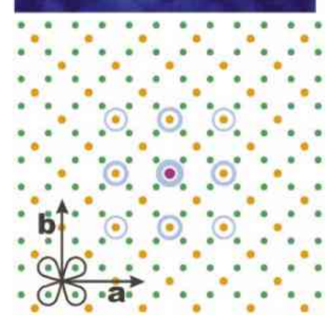
Stamp, Journal of Magnetism and Magnetic Materials, **63**, 429 - 431 (1987) (p-wave)

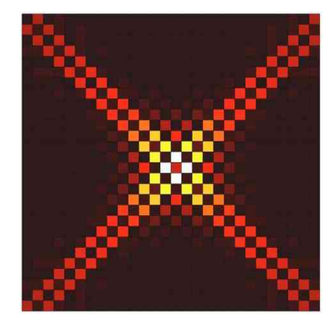
- Comparison to experiment



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







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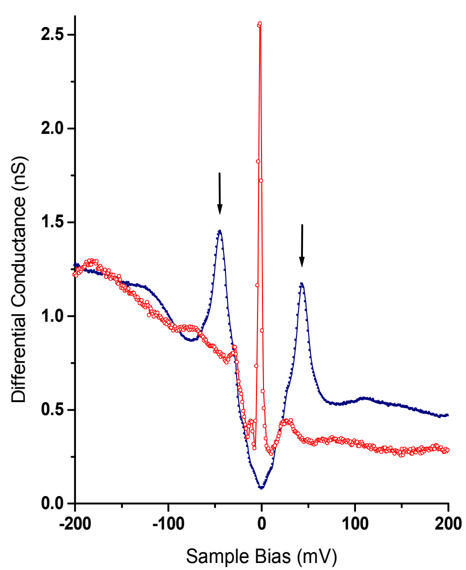
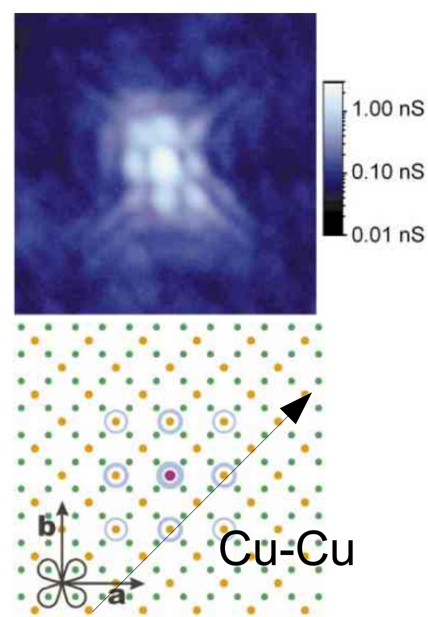
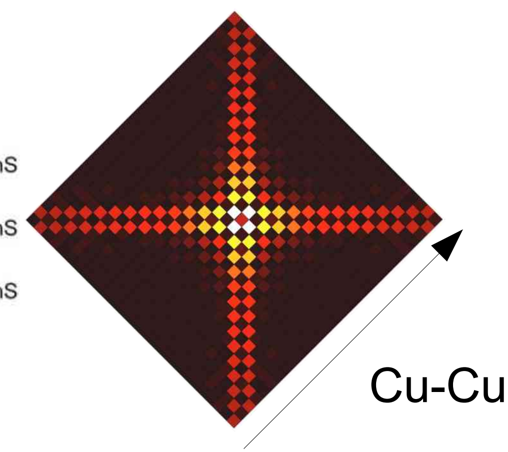


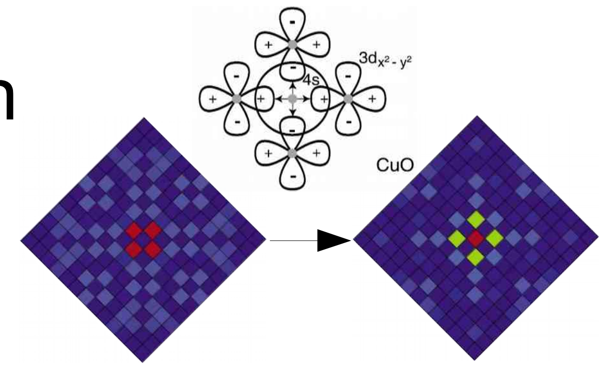
Pan et al., Nature **403**, 746 (2000)





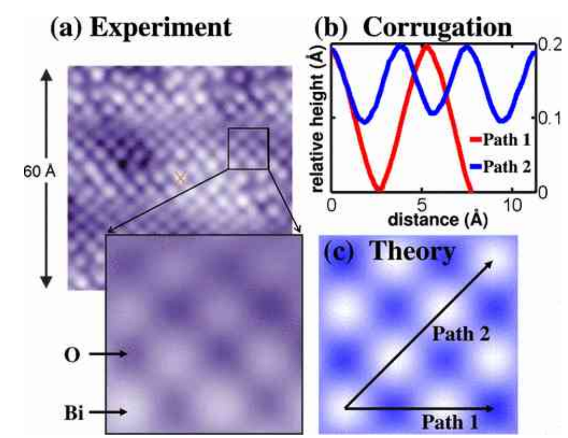
Theoretical approaches: Cuprates

- 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

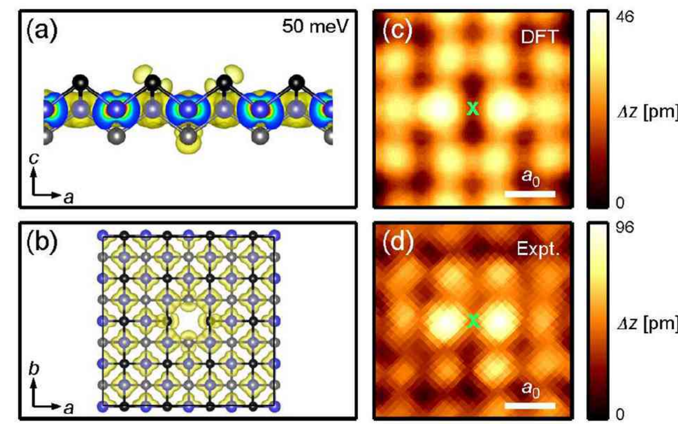
J. Nieminen, *et al.*, PRB **80**, 134509 (2009)



Theoretical approaches: Fe-SC

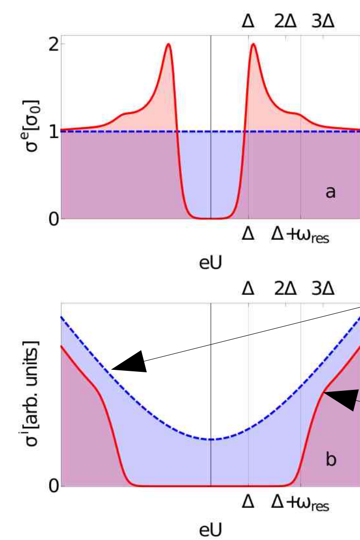
- Identification of nature of impurities in FeSe monolayer (non-SC) by ab-initio calculations

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



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

  S. Chi, *et al.*, Nat. Commun. **8**, 15996 (2017)



J. R. Kirtley and D. J. Scalapino, PRL **65**, 798 (1990); J. R. Kirtley, PRB **47**, 11379 (1993)
P. Hlobil, et al., Phys. Rev. Lett. **118**, 167001 (2017)

normal state

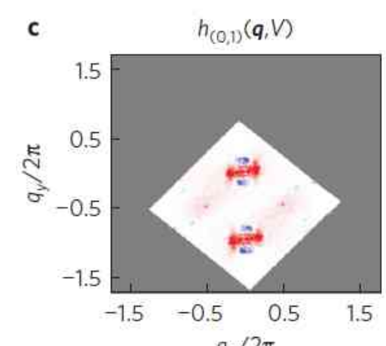
superconducting state

- 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

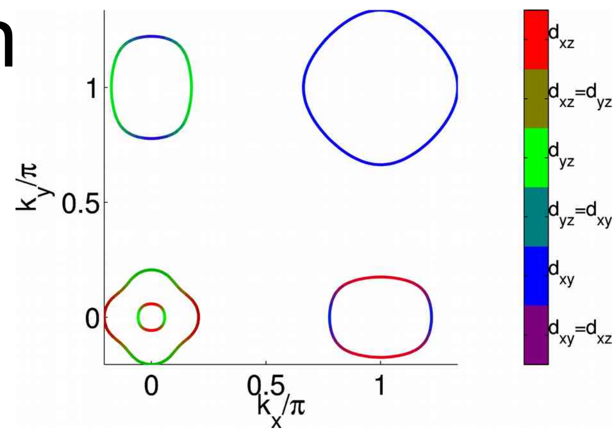


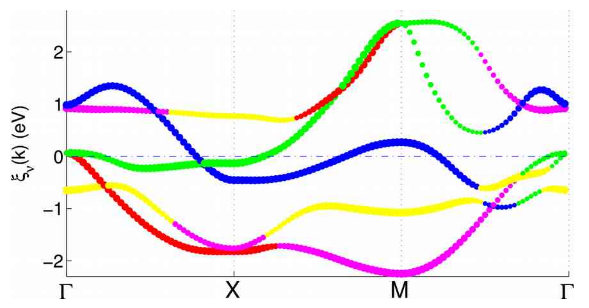
Wannier method: example LiFeAs

- Ab-initio calculation
  - band structure

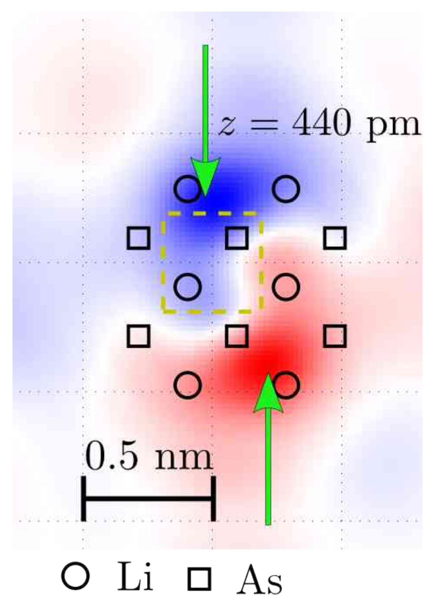
    5 band model

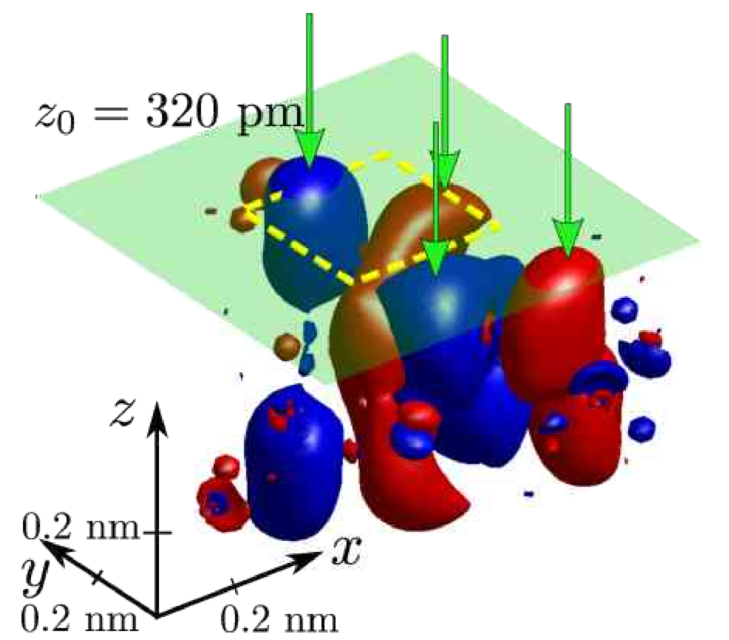
$$H_0 = \sum_{\mathbf{R}\mathbf{R}',\sigma} t_{\mathbf{R}\mathbf{R}'} c^\dagger_{\mathbf{R}\sigma} c_{\mathbf{R}'\sigma} - \mu_0 \sum_{\mathbf{R},\sigma} c^\dagger_{\mathbf{R}\sigma} c_{\mathbf{R}\sigma}$$





  - Wannier functions (including glide plane symmetry)





Superconductivity

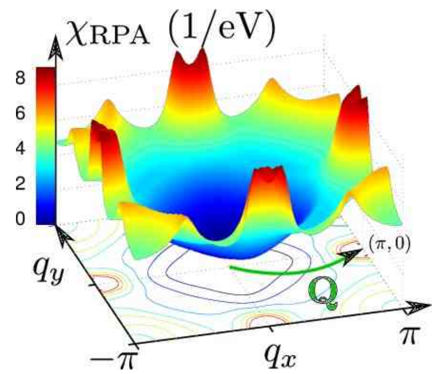
- superconducting order parameter from spin- fluctuation theory

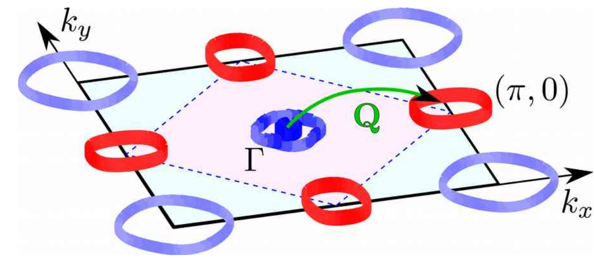
$$H_{\mathrm{BCS}} = -\sum_{\mathbf{R},\mathbf{R}'} \Delta_{\mathbf{RR}'} c^\dagger_{\mathbf{R}\uparrow} c^\dagger_{\mathbf{R}'\downarrow} + H.c.,$$

- calculate Green's function in superconducting state

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

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





Real space Greens function by Fourier transform

Impurity → engineered

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

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

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

- T-matrix approach to obtain Green's 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)

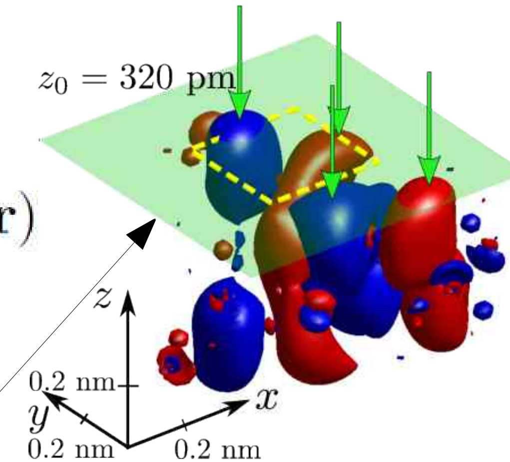
$$\underline{\hat{G}}_{\mathbf{R},\mathbf{R}'}(\omega) = \underline{\hat{G}}^{0}_{\mathbf{R}-\mathbf{R}'}(\omega) + \underline{\hat{G}}^{0}_{\mathbf{R}}(\omega)\underline{\hat{T}}(\omega)\underline{\hat{G}}^{0}_{-\mathbf{R}'}(\omega)$$

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

lattice Green function
(state of the art)

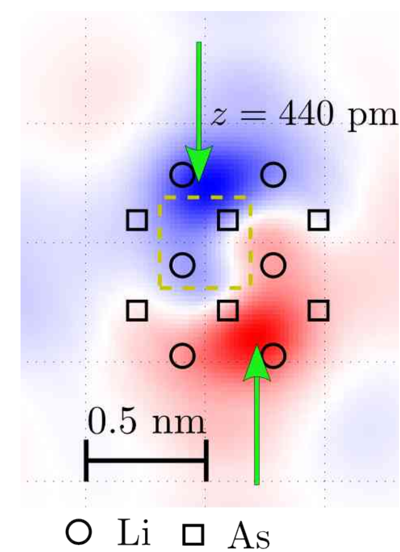
cLDOS

- 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

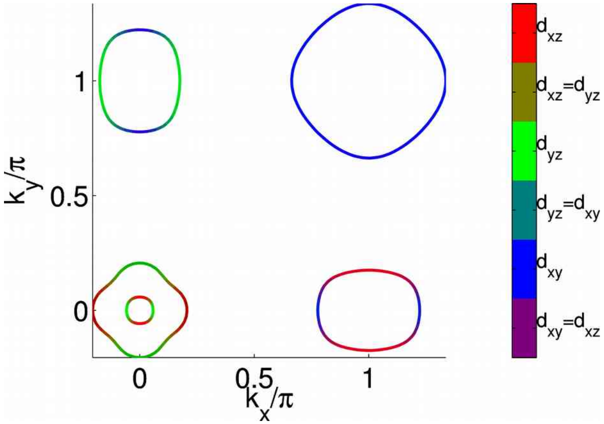
lattice Green function

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

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

LiFeAs: Questions

- Properties of the order parameter (sign-change)



conventional $s_{\pm}$

Y. Wang, A. Kreisel, et al., Phys. Rev. B **88**, 174516 (2013)
A. Kreisel, et al., Phys. Rev. B **95**, 174504 (2017)

antiphase $s_{\pm}$

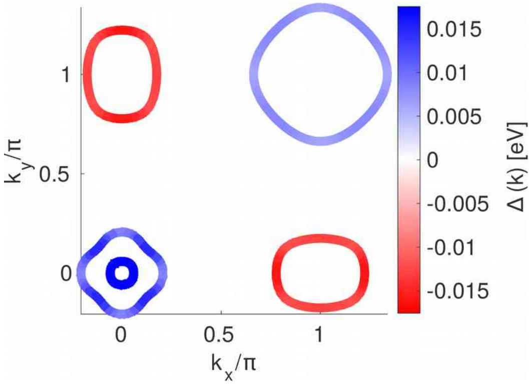
Z. P. Yin, K. Haule, G. Kotliar Nature Physics **10**, 845 (2014)

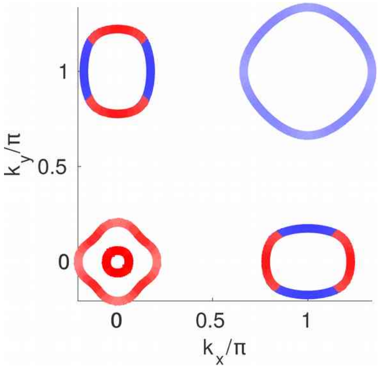
novel $s_{\pm}$

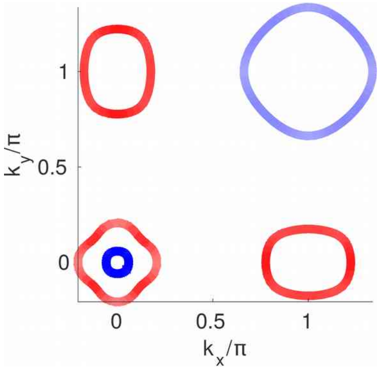
F. Ahn, et al., Phys. Rev. B 89, 144513 (2014)

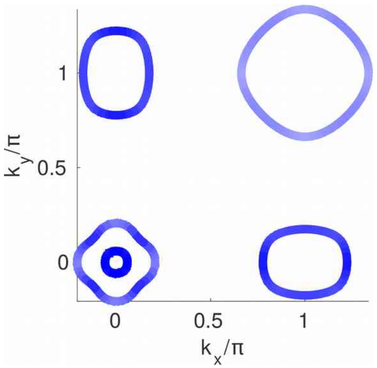
conventional s_{++}

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





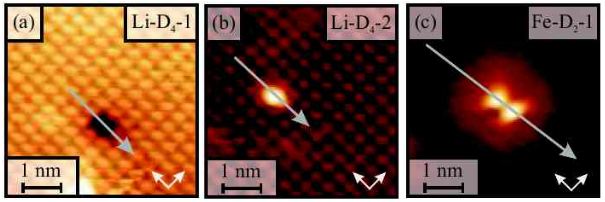




LiFeAs: Questions

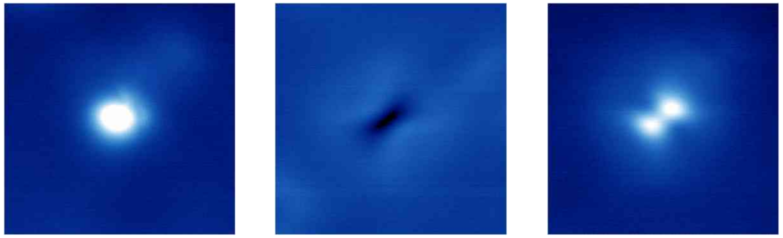
- Interpretation of
  - impurity shapes

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

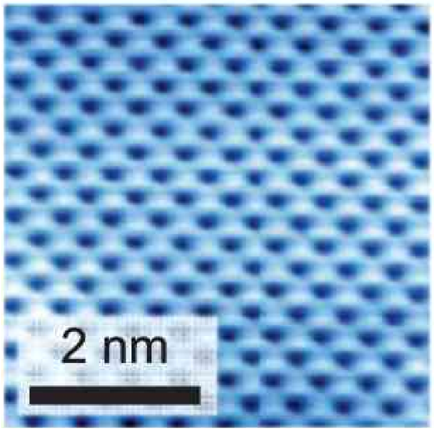


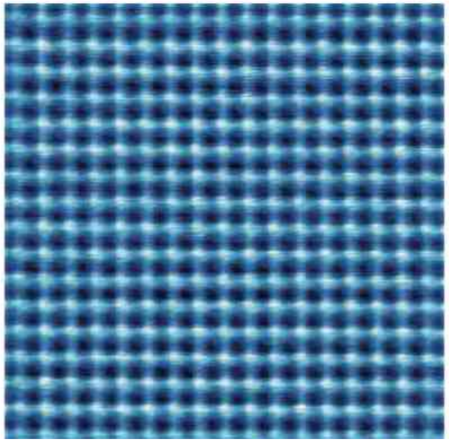
Hanaguri, unpublished (KITP 2011)

“Dot” “Trench” “Dumbbell”



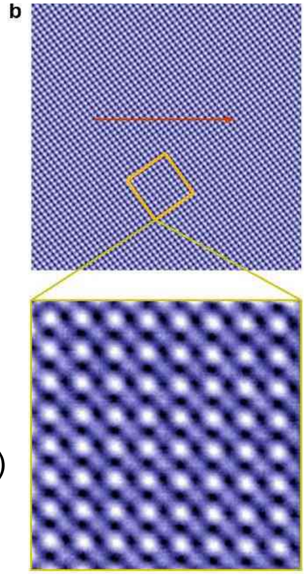
  - registered “surface lattice” in STM





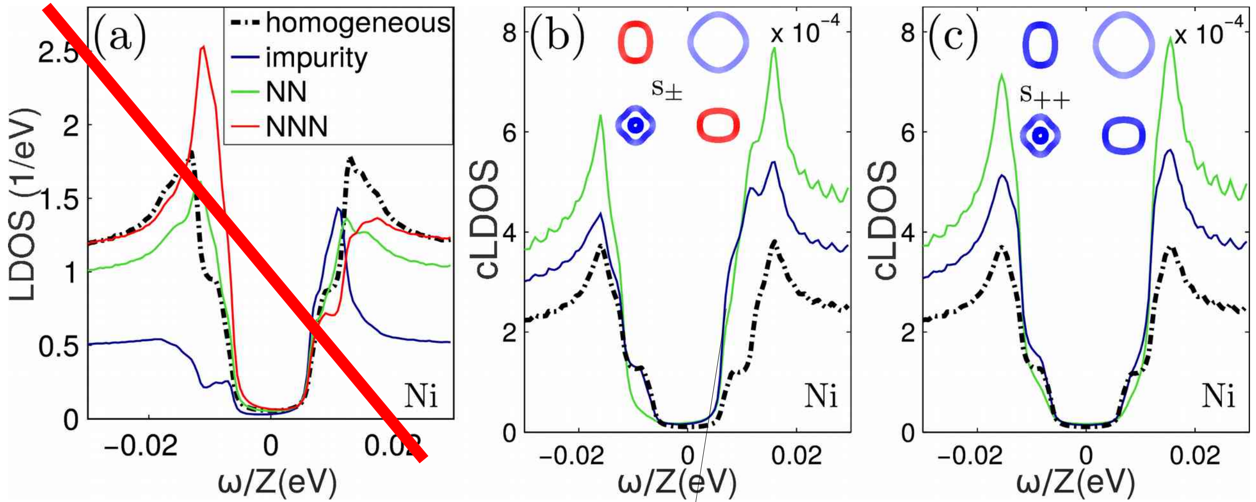
LiFeAs: Li or As lattice?

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)



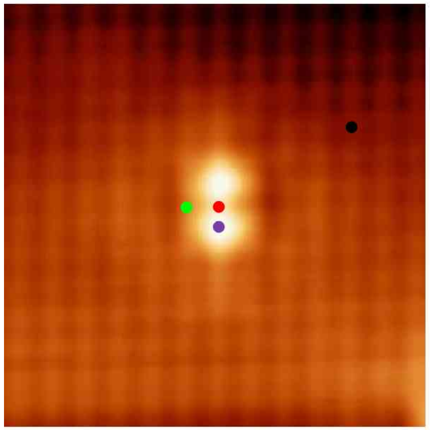
LiFeAs: spectra

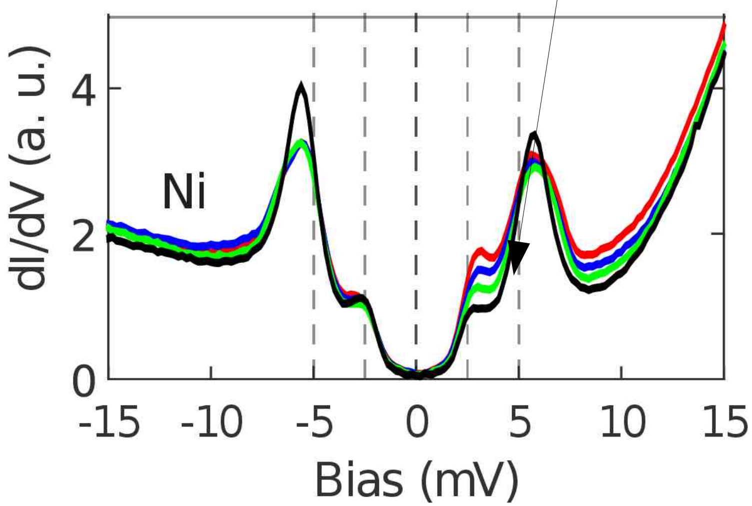
- evidence for sign-changing order parameter by in-gap state with engineered impurity



conventional calculation:
lattice LDOS: strong
response at negative bias

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

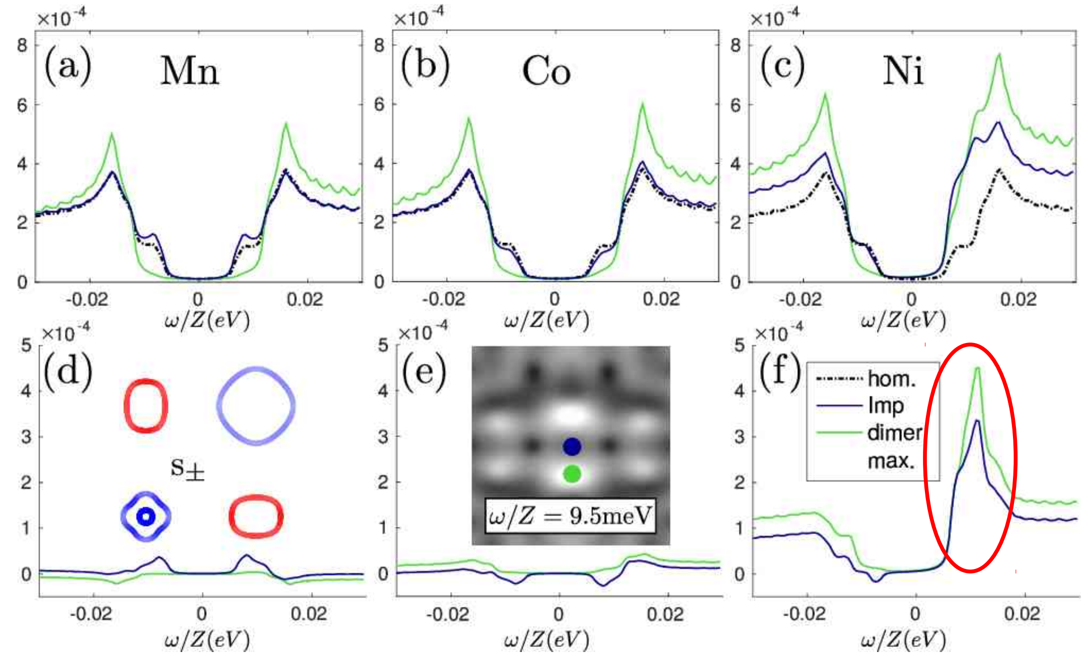


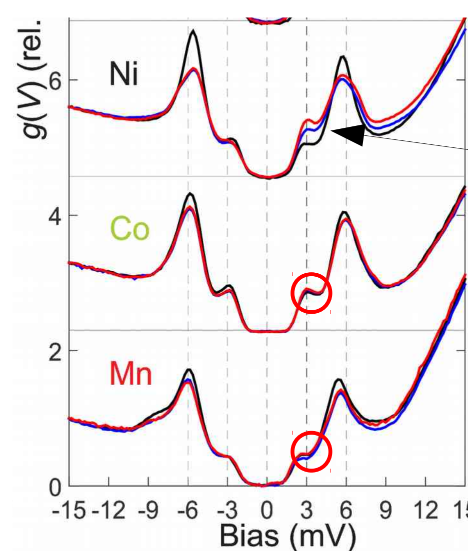


S. Chi, (...) , **A. Kreisel**, *et al.* Phys. Rev. B **94**, 134515 (2016)

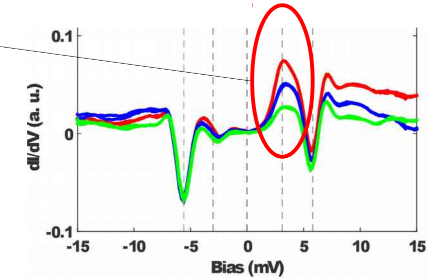
LiFeAs: spectra

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





relative spectra
Ni impurity



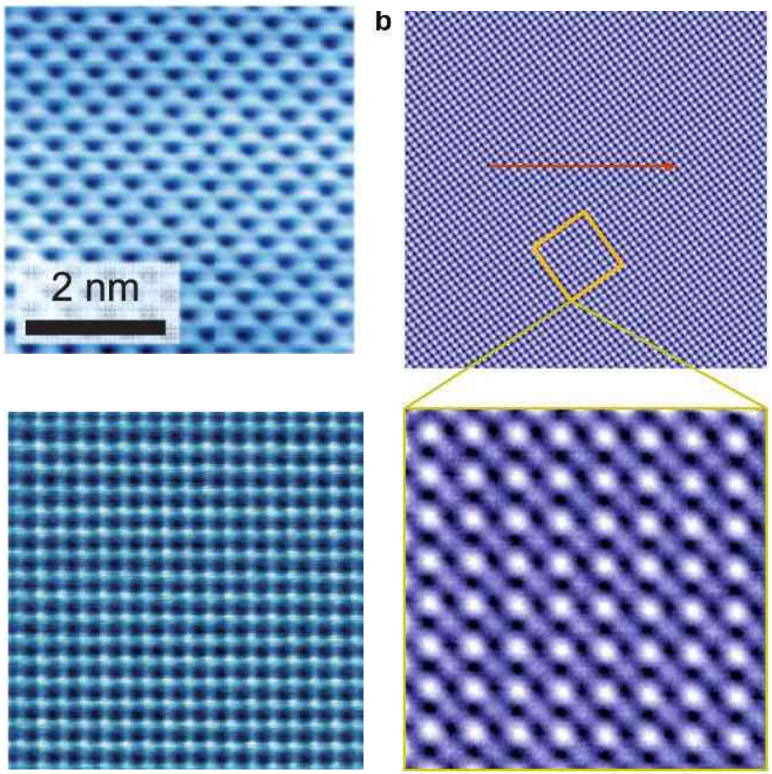
P. O. Sprau, …, A. Kreisel, et al., Science, **357**, 75 (2017)
A. Kreisel, et al., Phys. Rev. B **95**, 174504 (2017)
A. Kostin, et al., arXiv:1802.02266

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

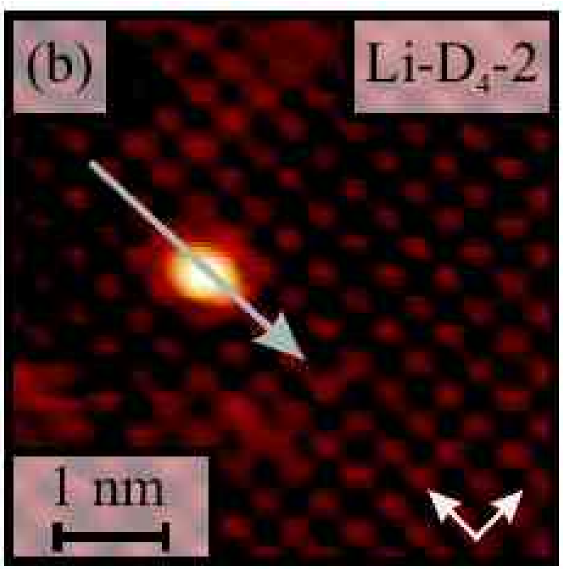
Height and current dependence of topographs

- experiment: Li or As lattice?

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



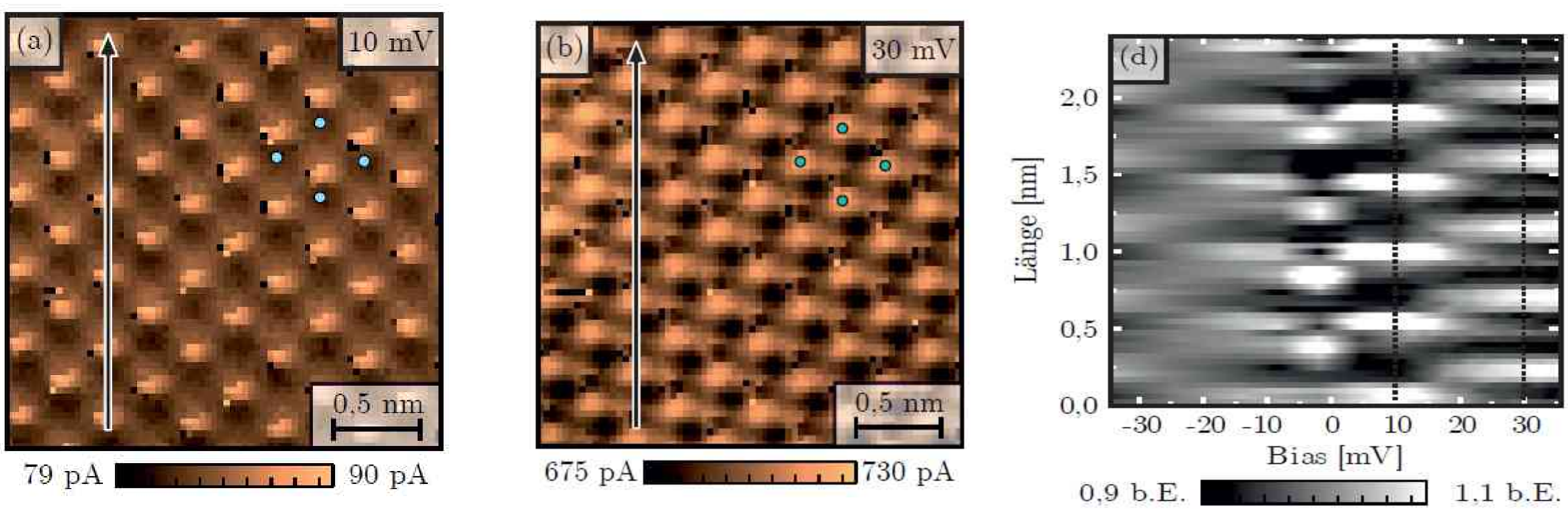
Shun Chi, et al., PRL 109, 087002 (2012)
T. Hanaguri, et al. PRB 85, 214505 (2012)
S. Grothe, et al., PRB 86, 174503 (2012)
J. -X. Yin, et al., arXiv, 1602.04949 (2016)



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

Further experimental evidences?

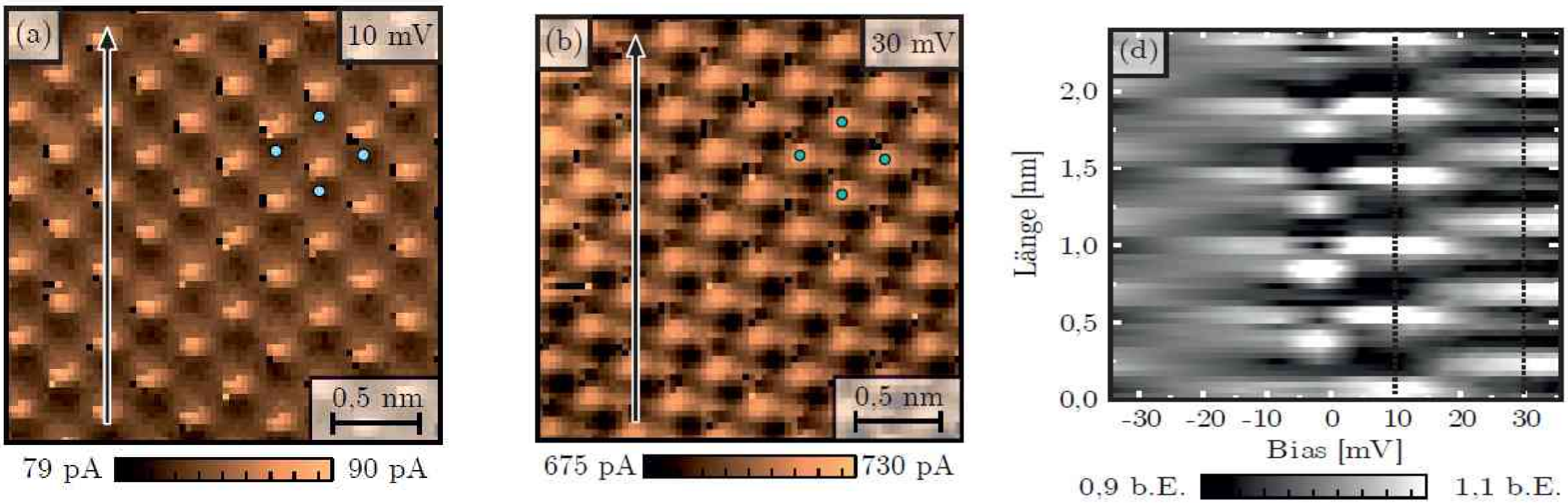
experiment (current maps)



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

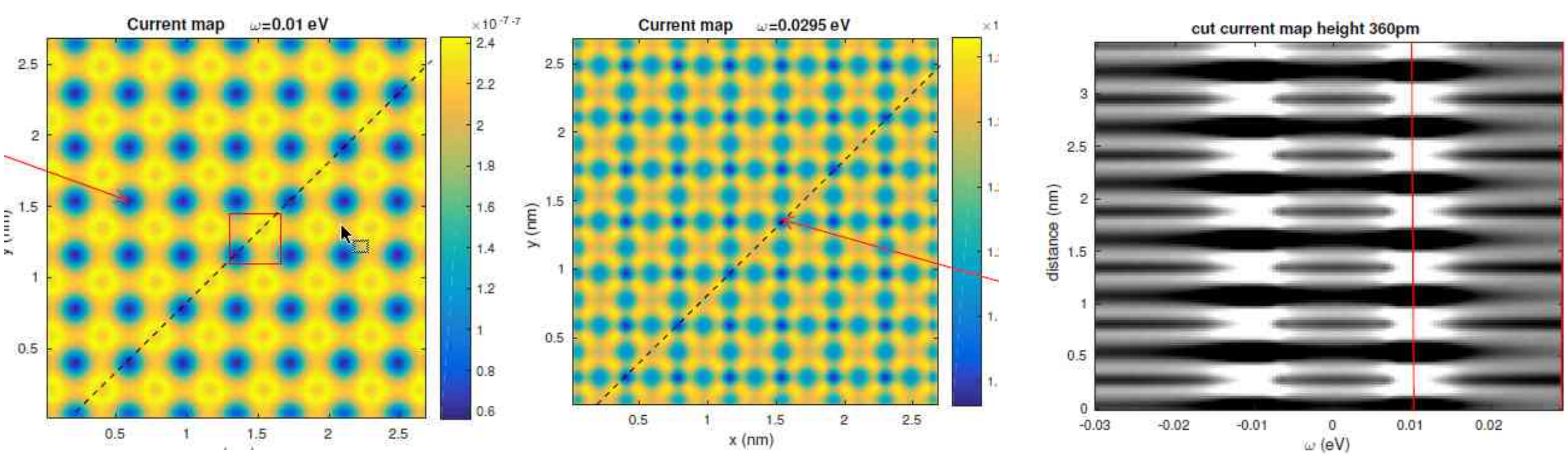
Further experimental evidences?

experiment (current maps)



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

theory

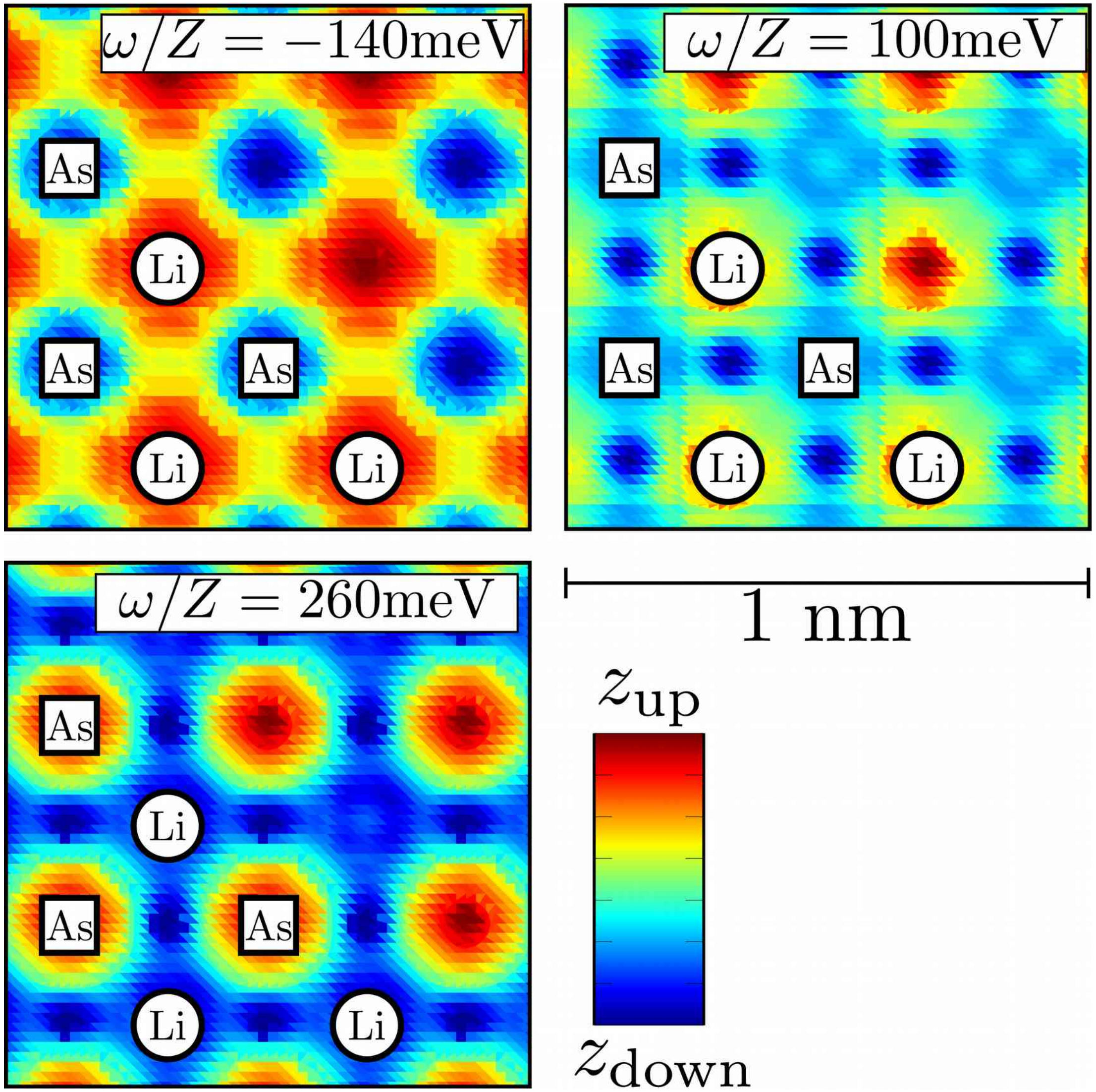


Simulation of topographs

- 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

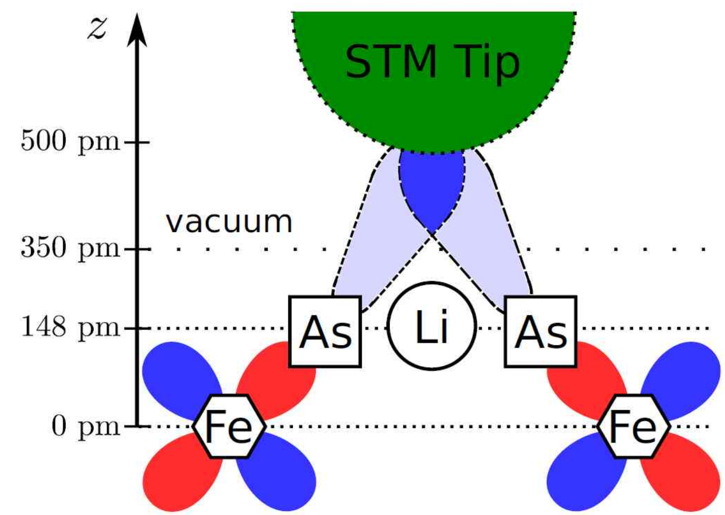


Results
registered surface lattice in STM

- tunneling into states described by Wannier functions

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

- registered lattice switches as function of bias and current

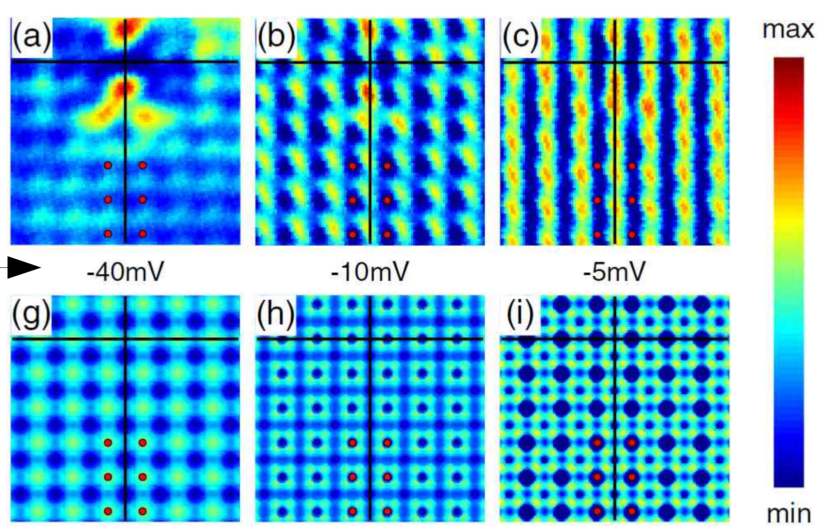


"Li lattice"   "As lattice"

measured topographies

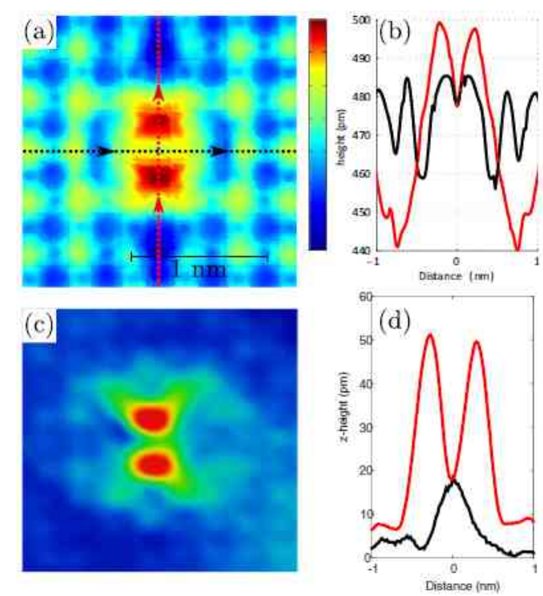
bias

simulated topographies



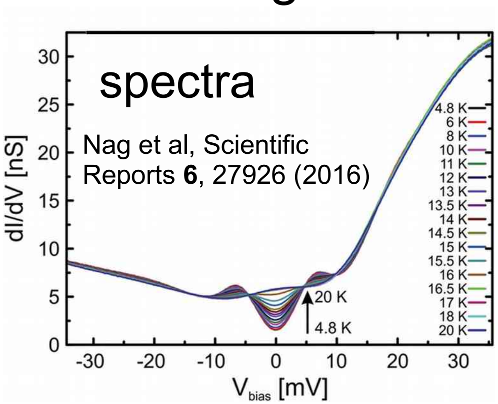
simulated topography close to strong imp.

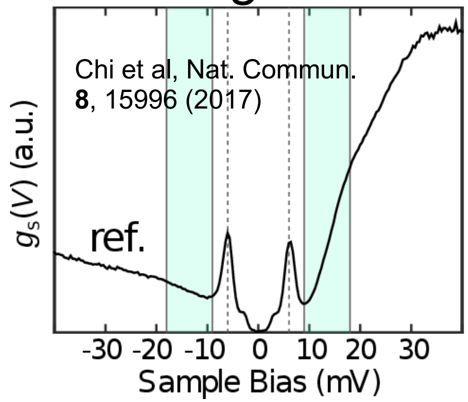
measured topography close to Ni

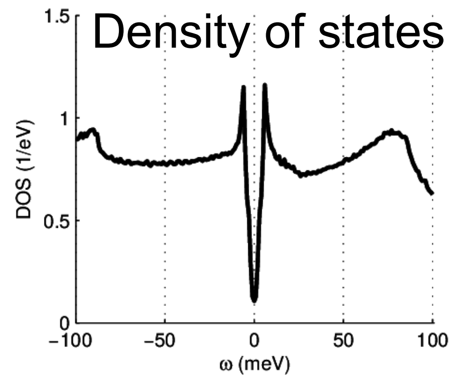


Inelastic tunneling

- well known property
  increasing conductance at large bias





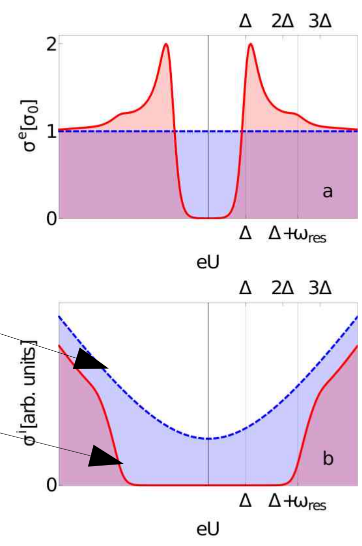


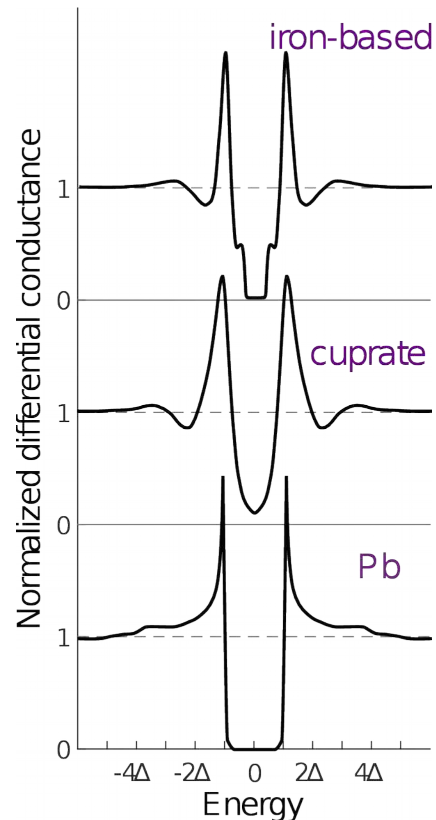
- deduction of collective modes?

$$g_{\rm tot}(\omega) = g_{\rm el}(\omega) + g_{\rm inel}(\omega)$$

normal state

superconducting state





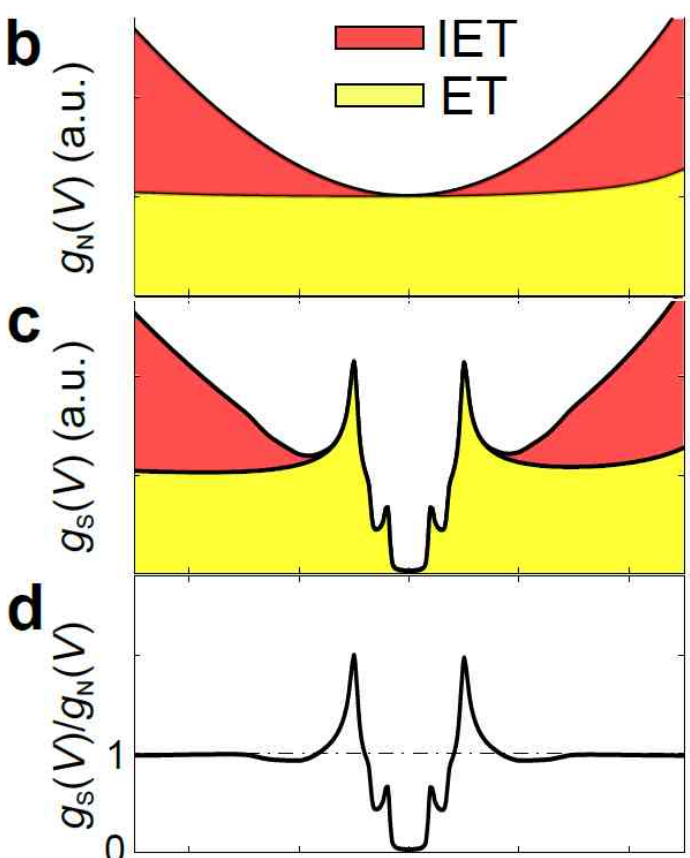
J. R. Kirtley and D. J. Scalapino, PRL **65**, 798 (1990); J. R. Kirtley, PRB **47**, 11379 (1993)
P. Hlobil, et al., Phys. Rev. Lett. **118**, 167001 (2017)

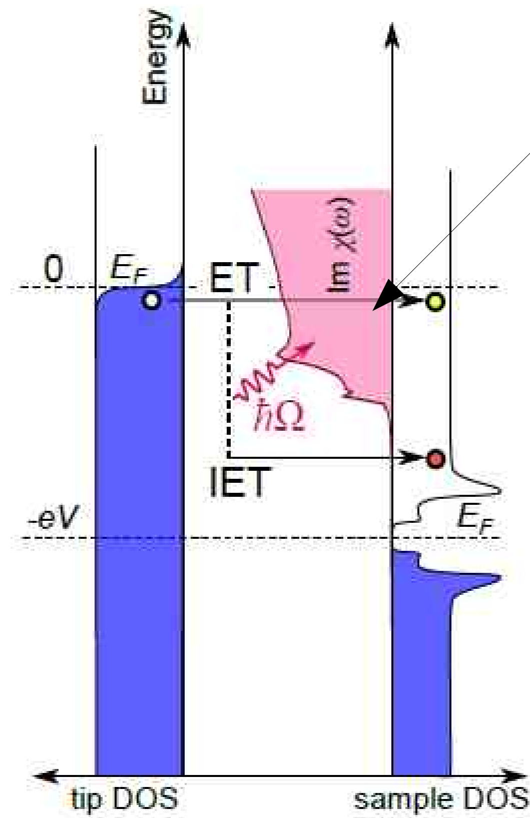
Inelastic tunneling in FeSC: coupling to spin fluctuations

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

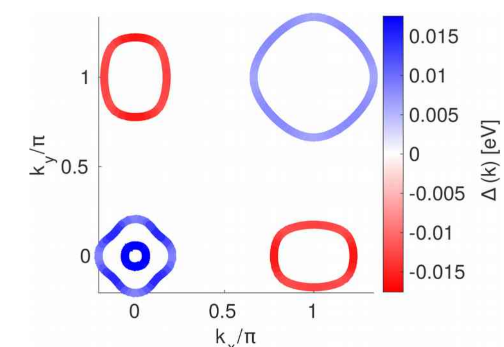
Spin fluctuations: two gap superconductor (LiFeAs), double resonance

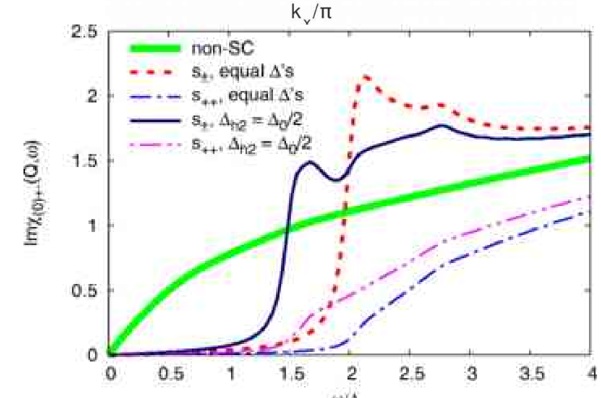
- Dip-hump feature





J. R. Kirtley and D. J. Scalapino, PRL **65**, 798 (1990); J. R. Kirtley, PRB **47**, 11379 (1993)
P. Hlobil, et al., Phys. Rev. Lett. **118**, 167001 (2017)





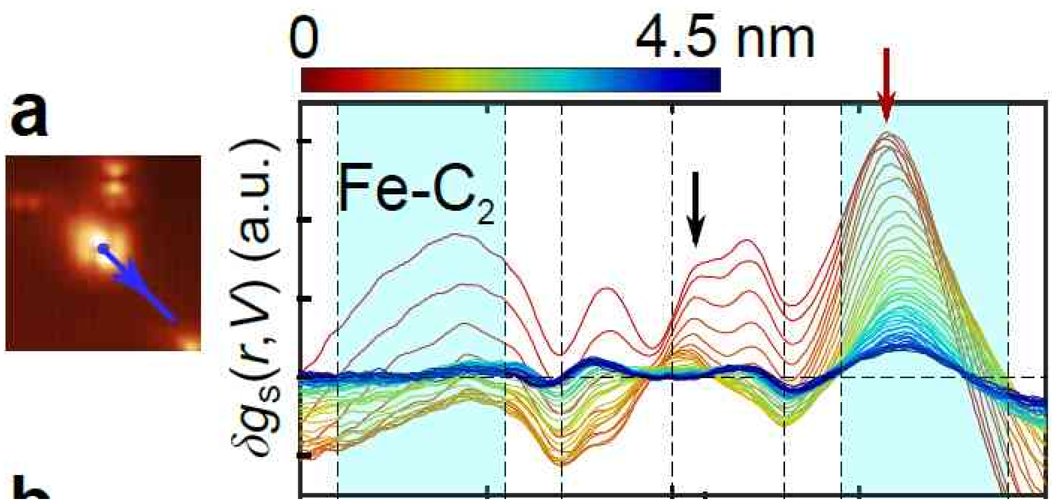
M. M. Korshunov, et al., Phys. Rev. B **94**, 094517 (2016)

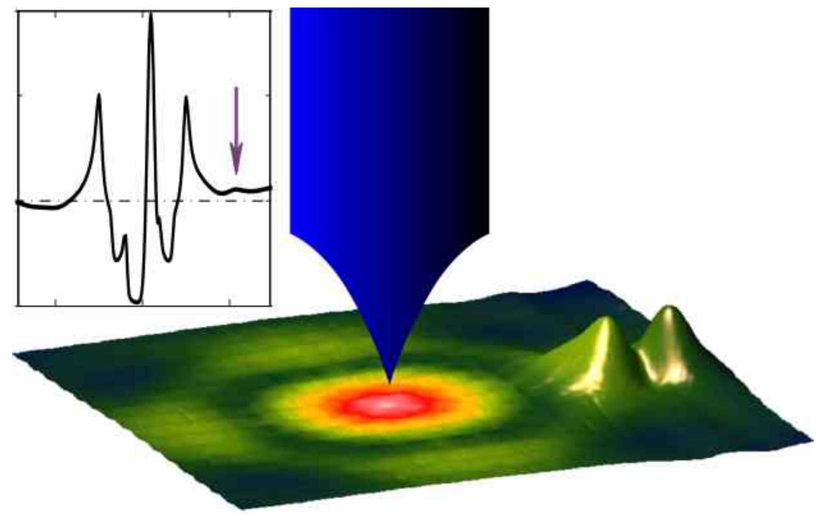
Imaging spin fluctuations in real space

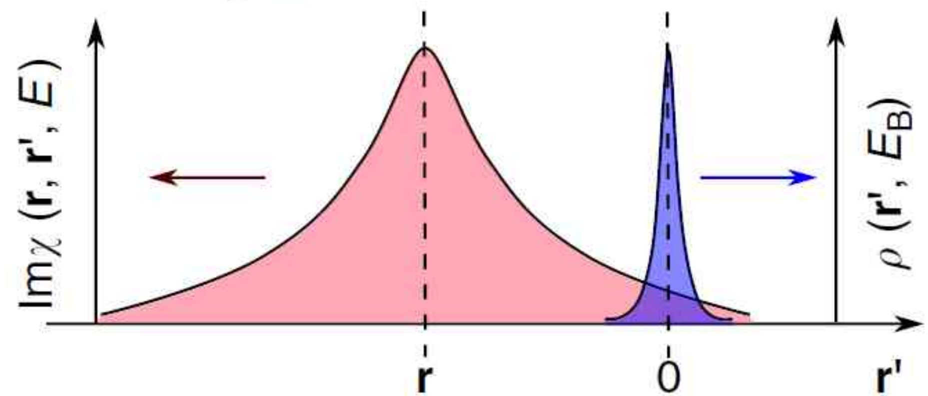
- real space structure $g_{\mathrm{inel}}(\mathbf{r}, V) \propto \int_0^{eV} \int \rho(\mathbf{r}', eV - \omega)\chi(\mathbf{r}, \mathbf{r}', \omega)\mathrm{d}\mathbf{r}'\mathrm{d}\omega$

S. Chi, (…) AK, et al., Nat. Commun. **8**, 15996 (2017)

- in presence of impurity



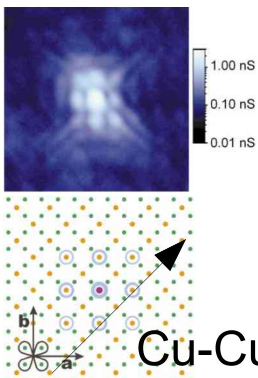


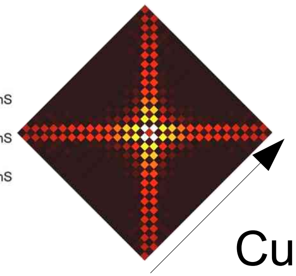


Fast spatial decay of impurity resonance, slow decay of dip-hump → spin fluctuations (real space)

Cuprates: Questions

- signatures of strong impurity in d-wave SC



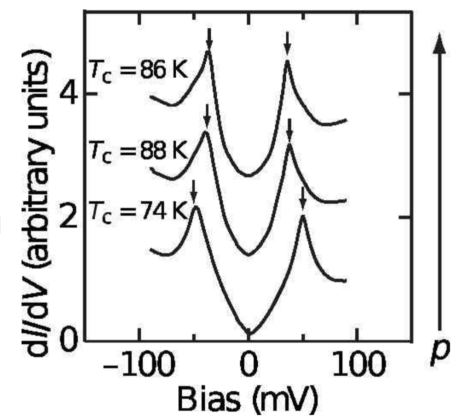


Cu-Cu

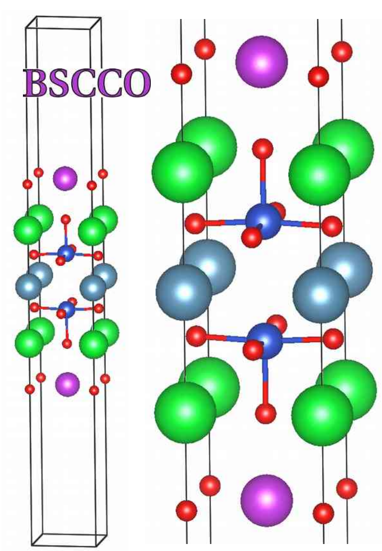
Cu-Cu

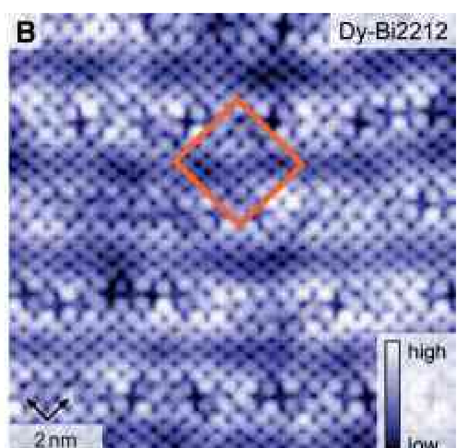
Kohsaka et al. Nature, **454**, 1072 (2008)

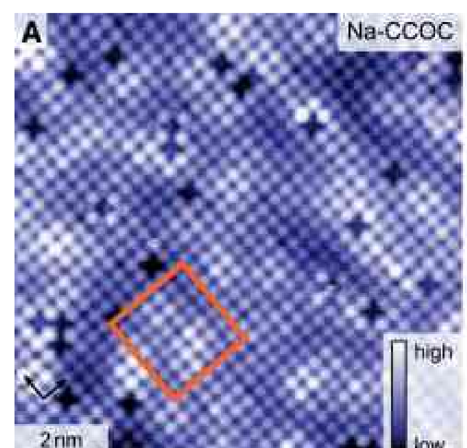
Crossover between U-shaped and V-shaped spectra

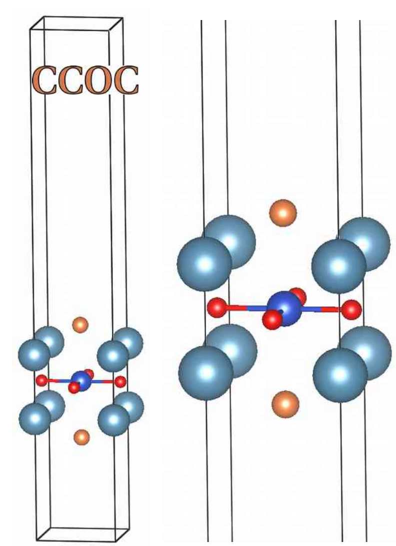


- universalities across materials







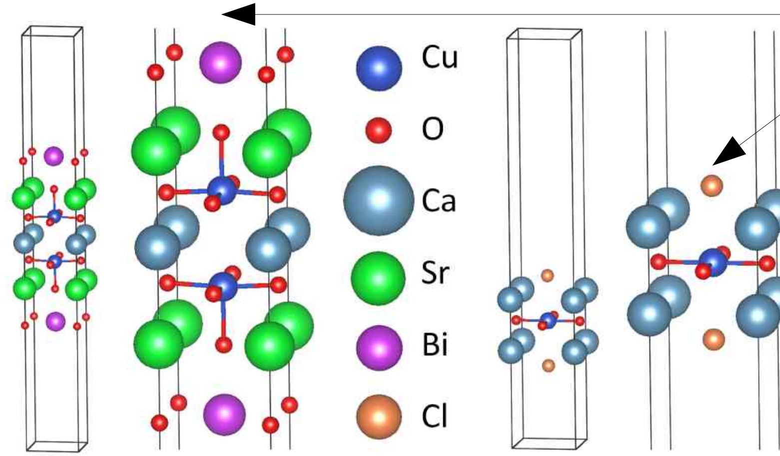


same properties for tunneling!

Wannier method: Cuprates

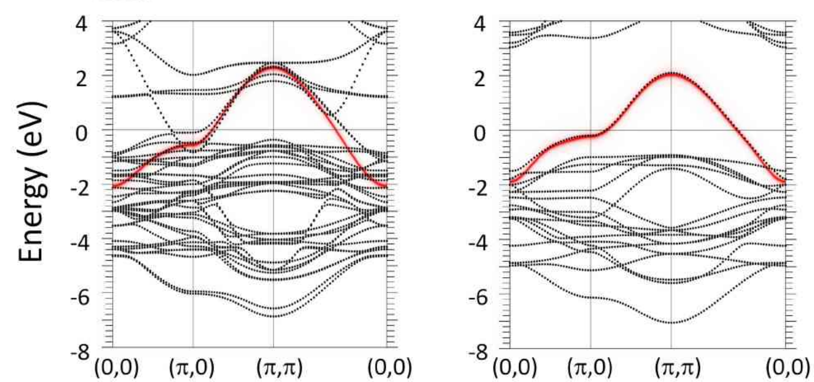
Surface
BiO vs. CaCl
and tunneling path
very different

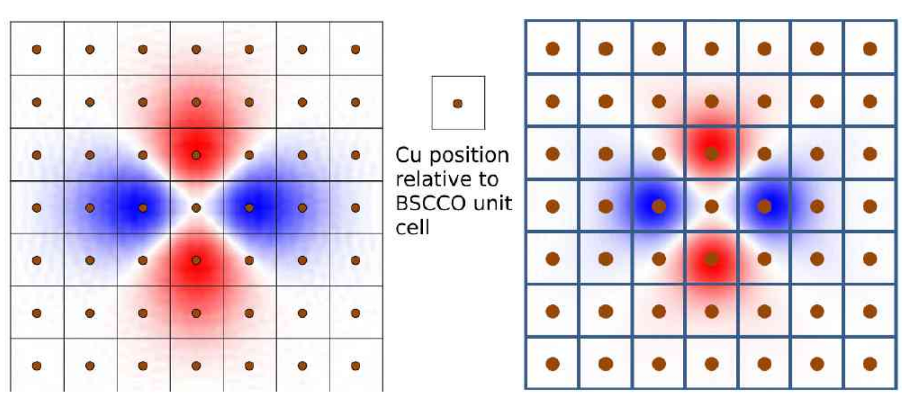
$Bi_2Sr_2CaCu_2O_8$



$Ca_2CuO_2Cl_2$

Ab initio calculation:
1 band model
+Wanner function

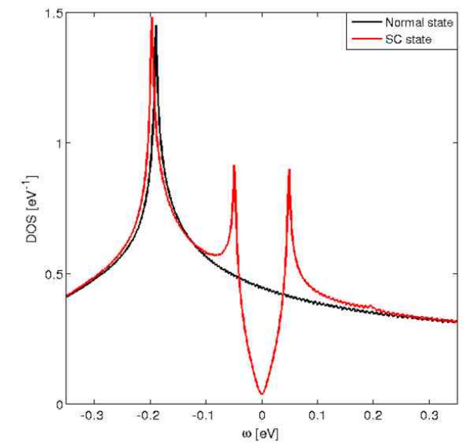




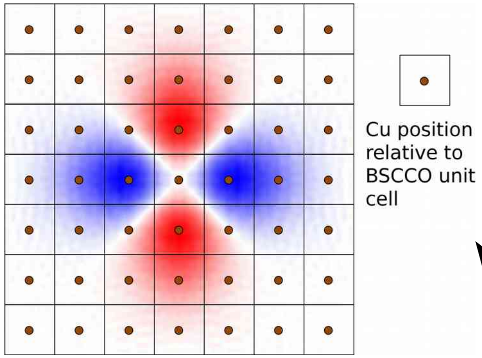
similar properties
dictated by
crystal symmetry

Superconductivity

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



- continuum Green function



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

surface Wannier function with phases

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

continuum position

nonlocal contributions

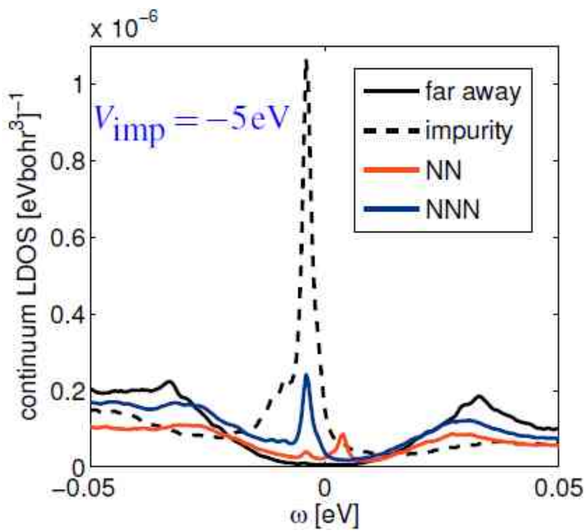
lattice Green function

local density of states (LDOS)

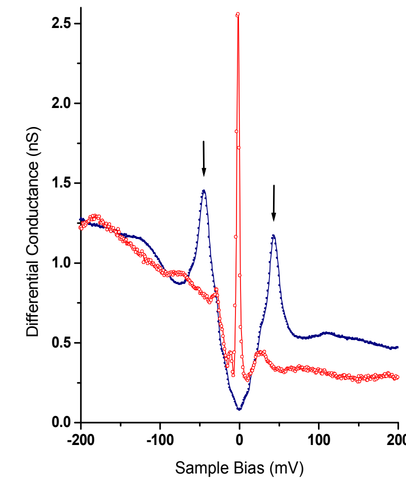
$$\rho(\mathsf{r},\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,G(\mathsf{r},\mathsf{r};\omega)$$

BSCCO: Results
STM maps and spectra

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

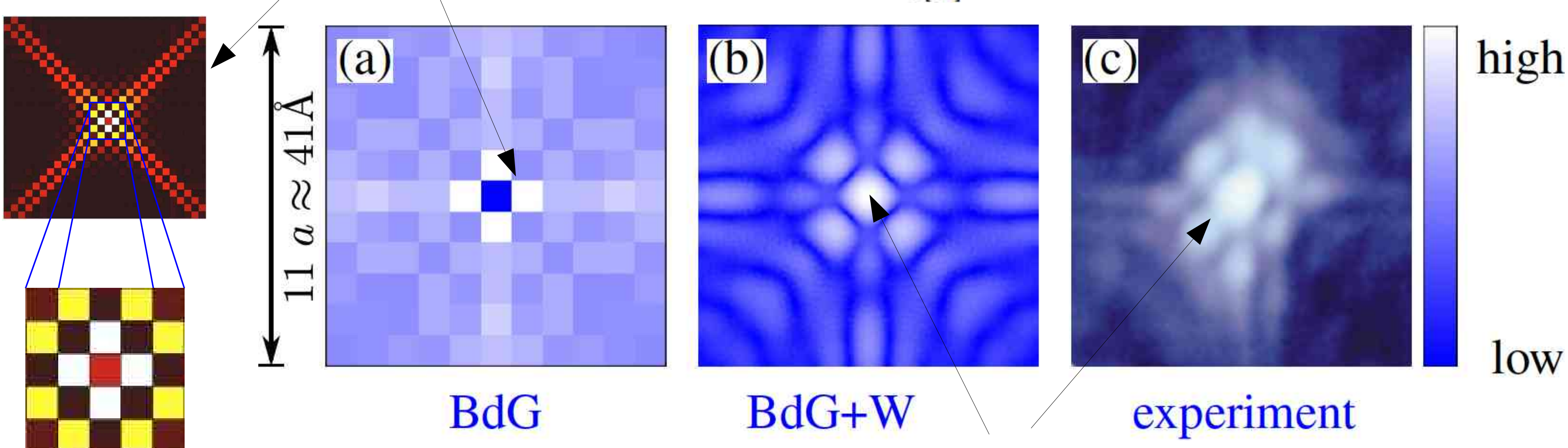


Pan et al., Nature **403**, 746 (2000)



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

resonance at NN

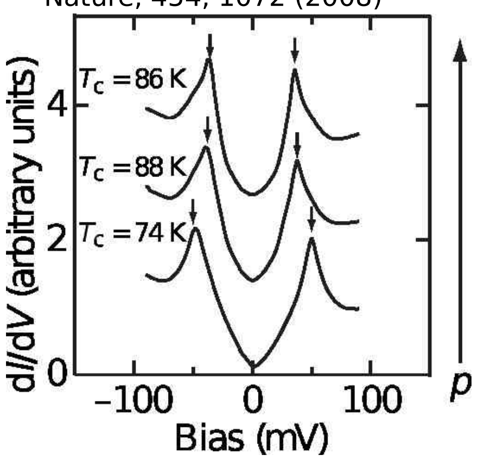


resonance at impurity

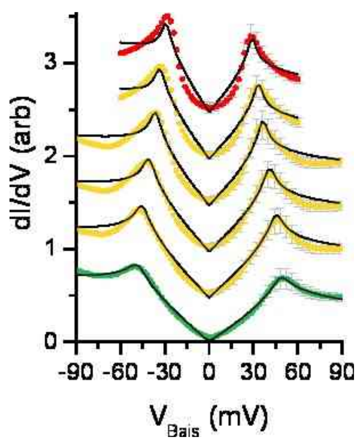
STM Spectra: homogeneous SC

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

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

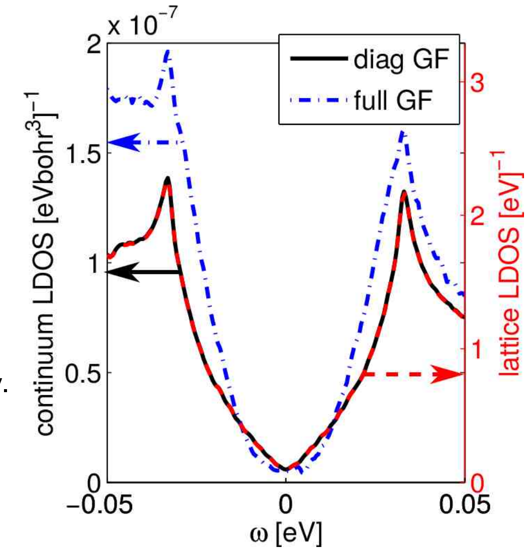


Alldredge et al.
Nature Physics, 4, 319 (2008)



BdG+W:
U-shape enters naturally within Wannier transformation

A. Kreisel, *et al.*, Phys. Rev. Lett. **114**, 217002 (2015)



- Analytical result
  - Spectral function
  - Wannier transformation
  - $d_{x^2-y^2}$ Wannier function
  - only cubic contribution

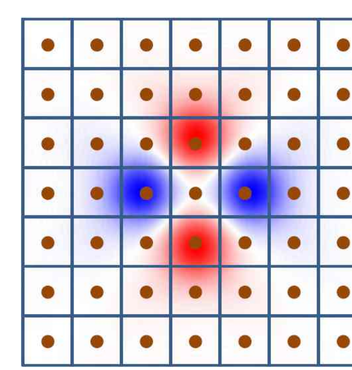
$$A_\sigma(\mathbf{k},\omega) = |u_\mathbf{k}|^2\delta(\omega - E_\mathbf{k}) + |v_\mathbf{k}|^2\delta(\omega + E_\mathbf{k})$$

$$\rho_\sigma(\mathbf{r},\omega) = \sum_\mathbf{k} A_\sigma(\mathbf{k},\omega)|W_\mathbf{k}(\mathbf{r})|^2$$

$$W_\mathbf{k}(\mathbf{r}_0) \approx w_0 + 2w_1(\cos k_x - \cos k_y)$$

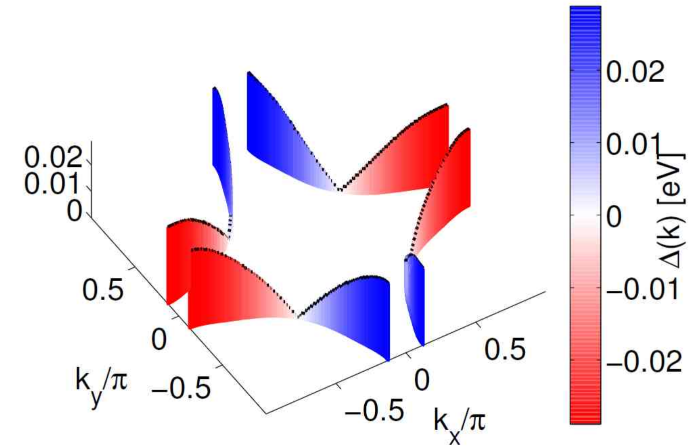
$$w_0 = 0$$

$$\rho_\sigma = w_1^2 \frac{4\sin^2(k_x^0)}{\pi^3 v_F v_\Delta^3}\omega^3$$



P. Choubey, *et al.*. Phys. Rev. B **96**, 174523 (2017)

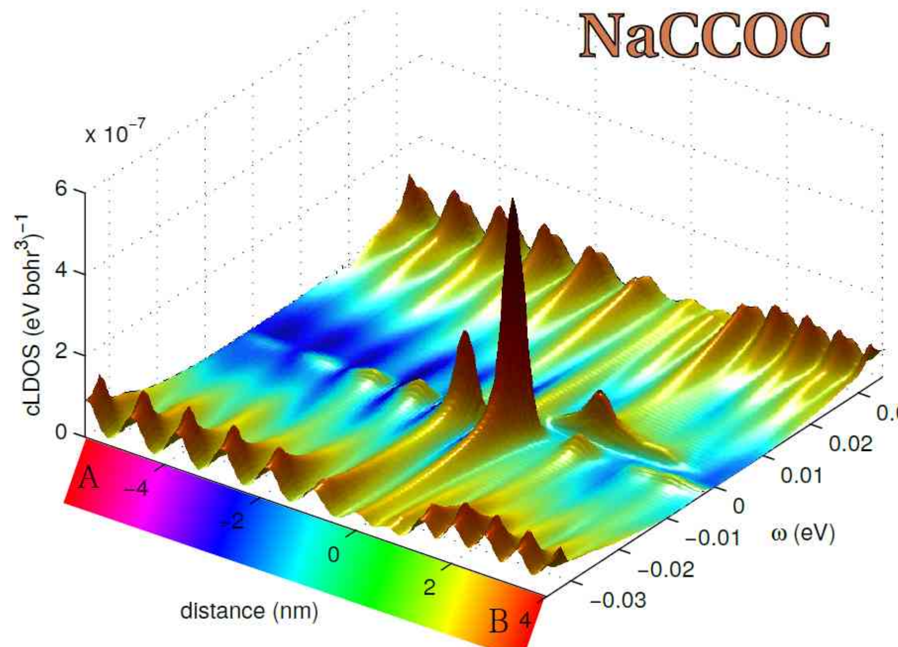
$Bi_2Sr_2CaCu_2O_8 \leftrightarrow Ca_2CuO_2Cl_2$

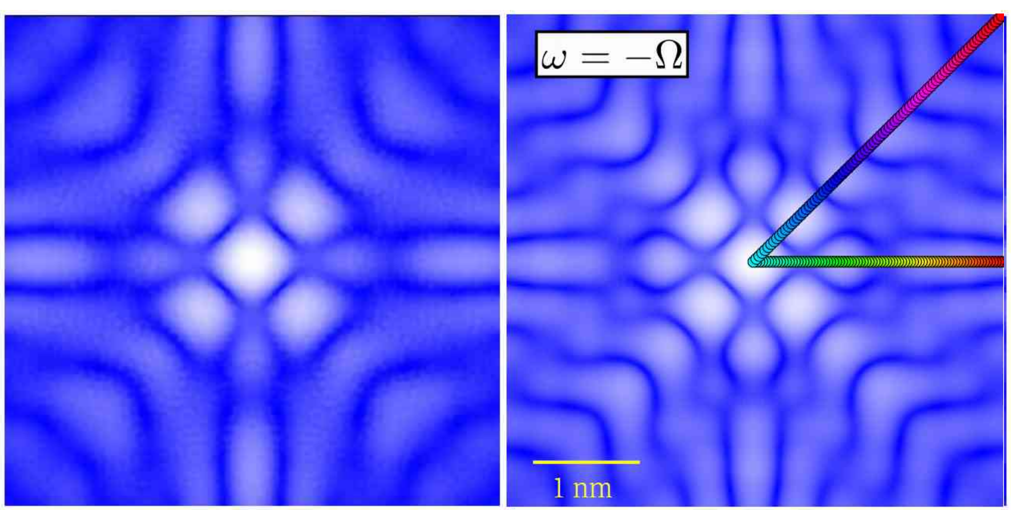


- superconductivity:
  d-wave order parameter
- T-matrix calculation+ Wannier method

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

- strong impurity
  spectra + conductance map





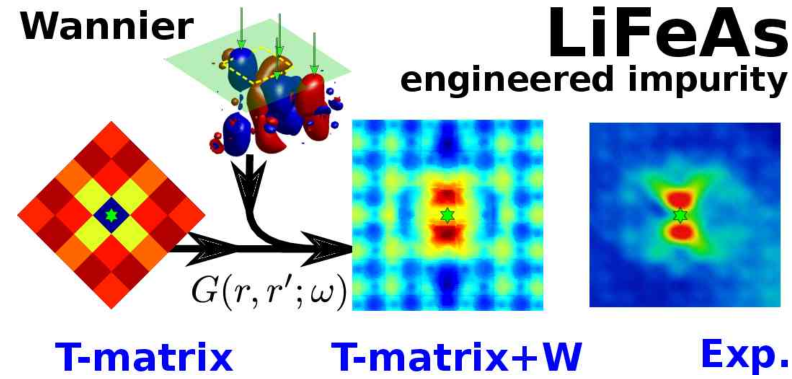
$Bi_2Sr_2CaCu_2O_8$ $Ca_2CuO_2Cl_2$

Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey et al., New J. Phys. **19**, 013028 (2017)
P. Choubey, *et al.*. Phys. Rev. B **96**, 174523 (2017)

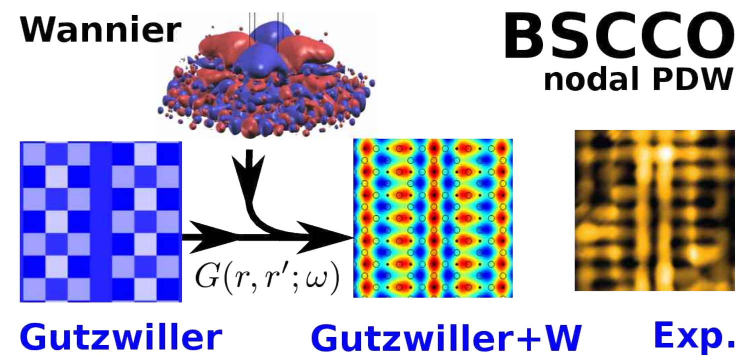
Summary

- Wannier method: basis transformation of the lattice Green function
- Qualitative correct (symmetry) and quantitative predictive results
- Impurities and homogeneous lattice in LiFeAs
- inelastic tunneling   S. Chi, (…) AK, et al., Nat. Commun. **8**, 15996 (2017)
- Universality in cuprates
- method to detect sign change of order parameter in STM
  Martiny, Kreisel, Hirschfeld, Andersen Phys. Rev. B **95**, 184507 (2017)
  Sprau, et al. Science, **357**, 75 (2017)
- Nematicity in Fe-based SC

  A. Kostin,et al., arXiv:1802.02266



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)
Choubey, *et al.*. Phys. Rev. B **96**, 174523 (2017)

Acknowledgments