Wannier based theory of unconventional superconductors

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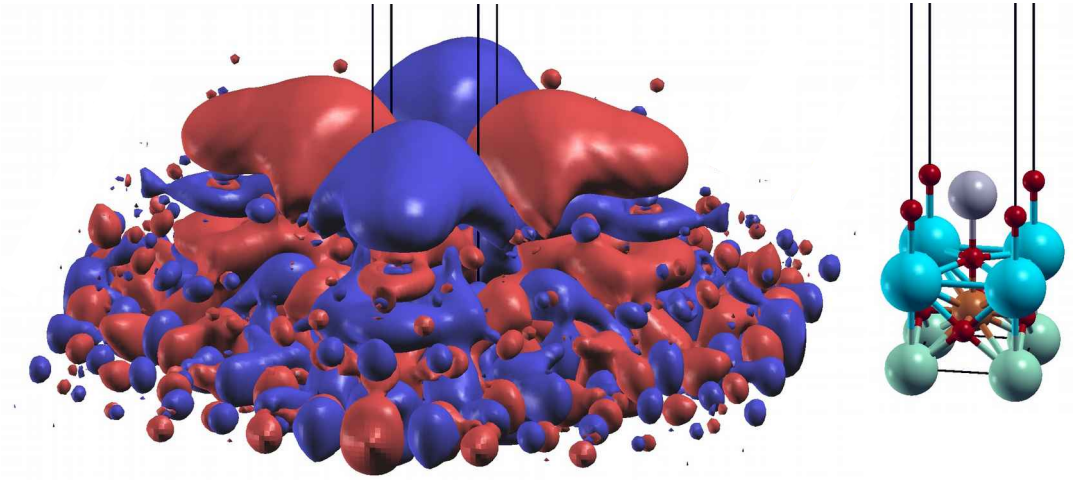

A. Kreisel, *et al.*, Phys. Rev. Lett. **114**, 217002 (2015)
A. Kreisel, *et al.,* Phys. Rev. B **94**, 224518 (2016)
P. Choubey, AK, et al. Phys. Rev. B **96**, 174523 (2017)

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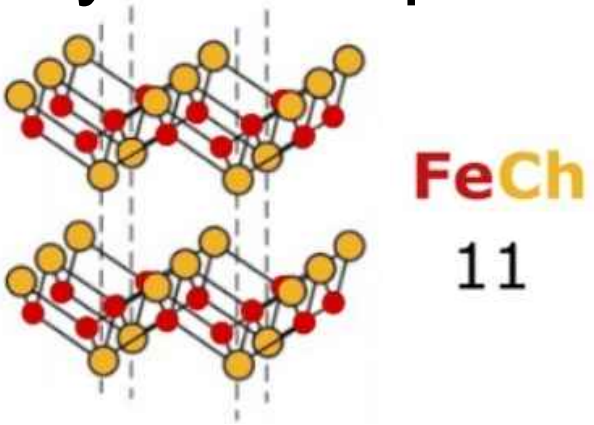
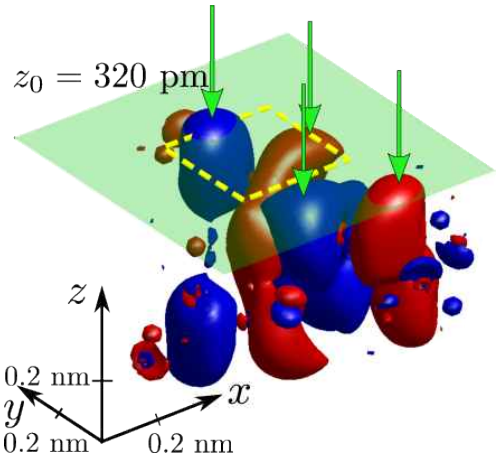
Theoretical simulation of STM

- Scope:layered superconductors, complications



- using wavefunction information in layered superconductors: Wannier method
  - Applications
    - LiFeAs (multiband, s-wave)
    - Cuprates: $Bi_2Sr_2CaCu_2O_8$, $Ca_2CuO_2Cl_2$
    - FeSe (nematic state, orbital order)



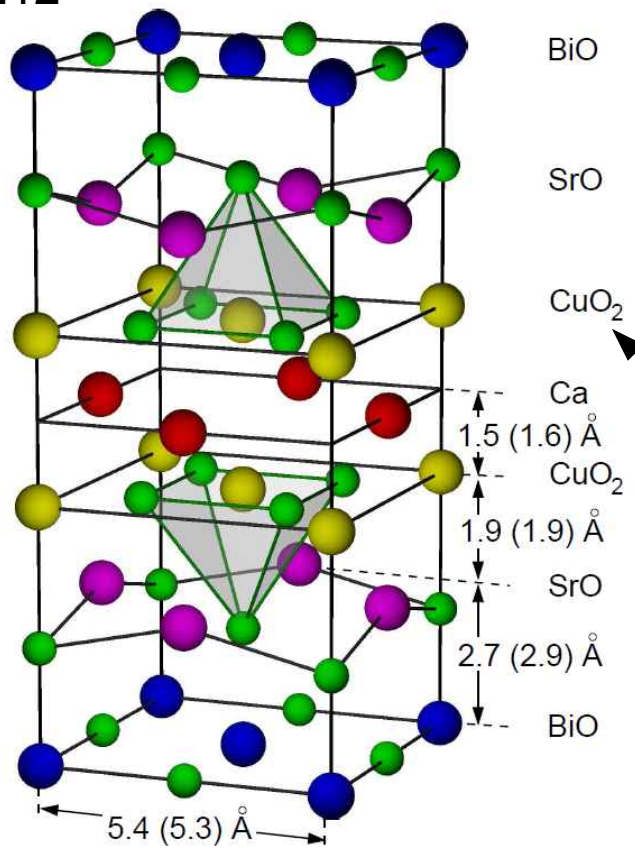
Layered superconductors

- 2 examples: surface atoms ≠ superconducting layer

Cuprates

Bi-2212

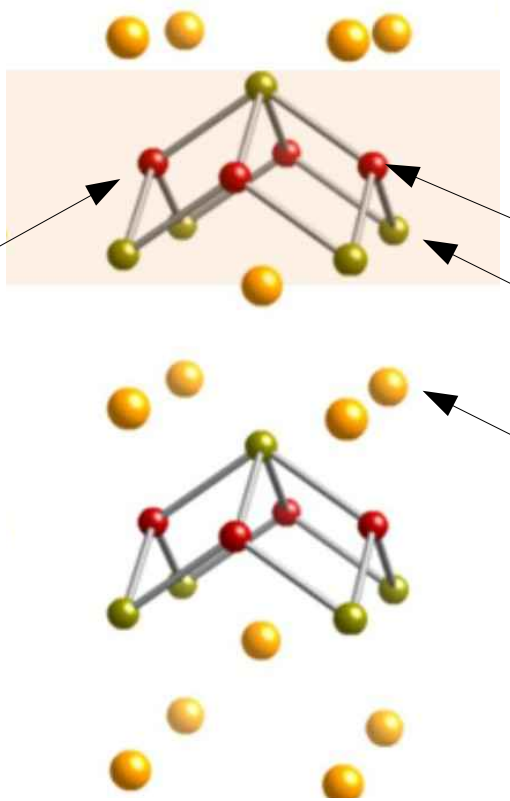
surface: BiO



states at the Fermi level
Cu-plane
Fe-plane

Iron based superconductors

surface: Li, As?



LiFeAs

"111"

Fe

As

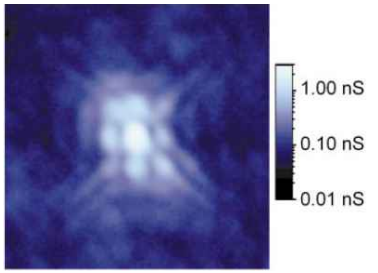
Li

Theoretical approaches: Cuprates

- LDOS: impurity in d-wave superconductor → bound state

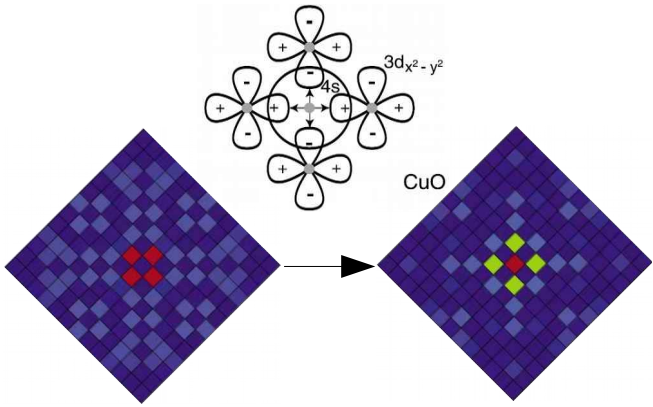
$$\Omega \equiv \Omega' + i\Omega'' = \Delta_0 \frac{\pi c/2}{\ln(8/\pi c)} \left[1 + \frac{i\pi}{2} \frac{1}{\ln(8/\pi c)}\right]$$

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)



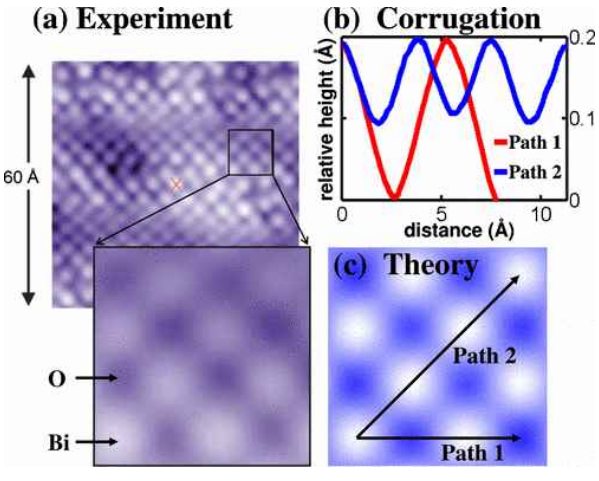
- "Filter function": STM tip probes states in the superconducting layer by tunneling matrix elements

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)



Approaches: multiband systems

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

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

- Ab initio calculations of effects of orbital order on the surface layer

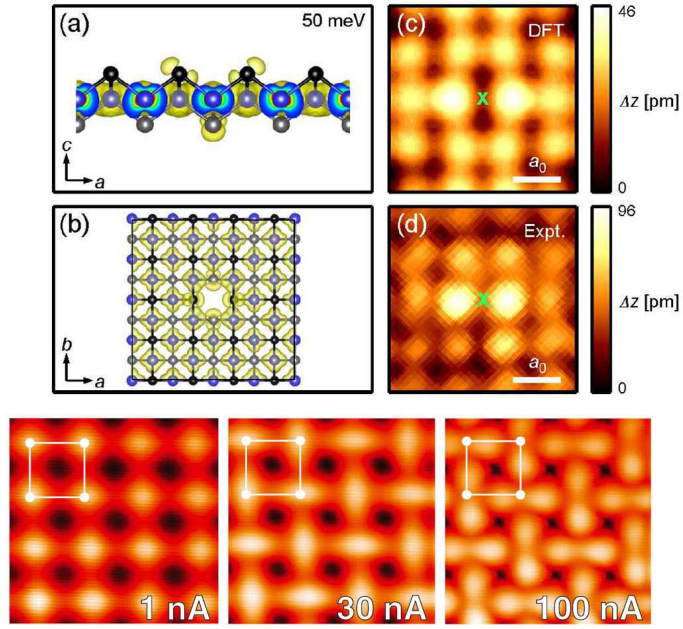
  Kim et al., Sci. Adv. 2017; **3**: eaao0362

- Wannier method (this talk)

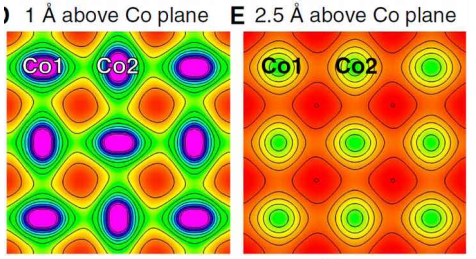
See also: “holographic maps”
Dalla Torre, He, Demler
Nat. Phys., **12**, 1052 (2016)

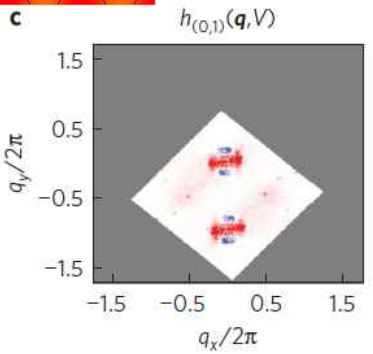
$$h_G(q,V) = g(q,V)g^*(q+G,V)$$

unravel intra-unitcell information



CeCoIn5





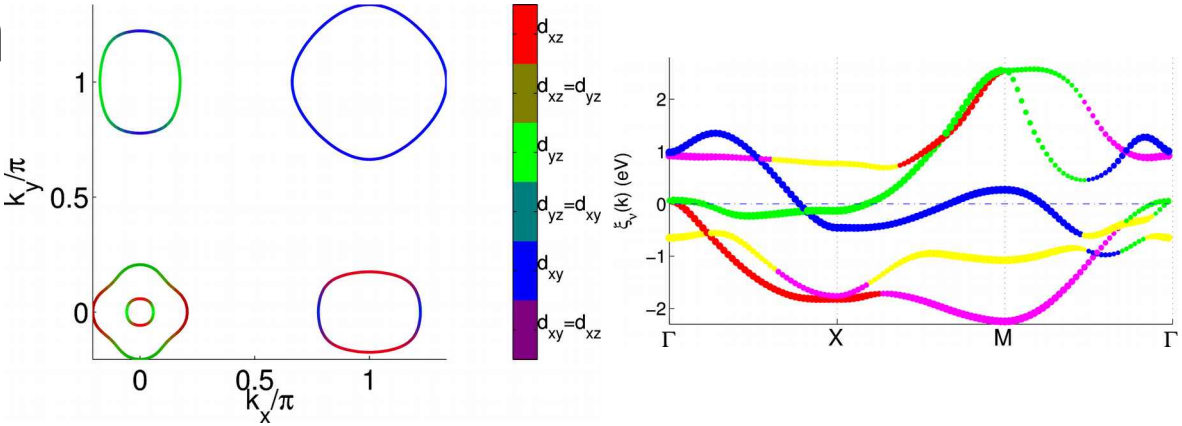
Wannier method: example LiFeAs

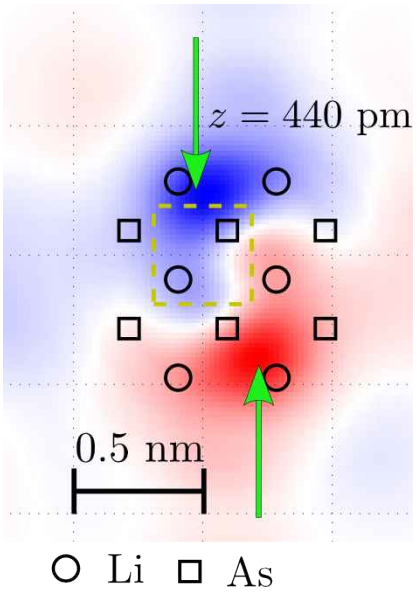
- Ab-initio calculation
  - band structure

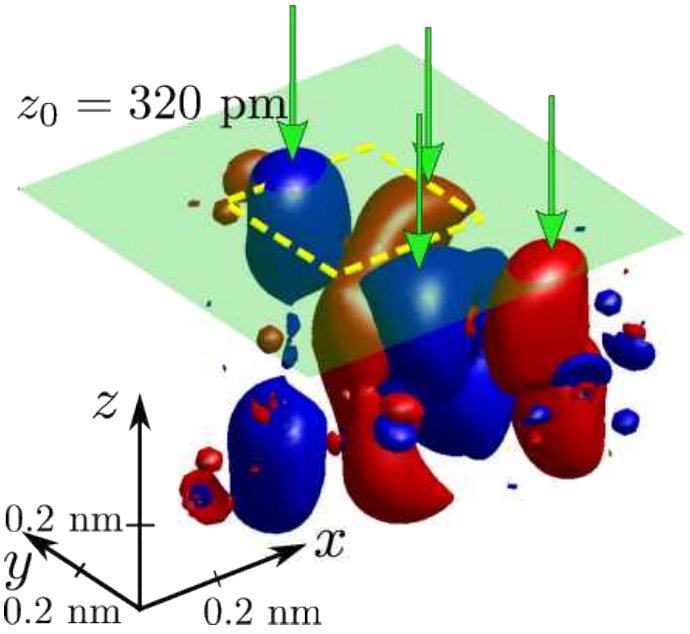
    5 band model

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

  - Wannier functions (including glide plane symmetry)



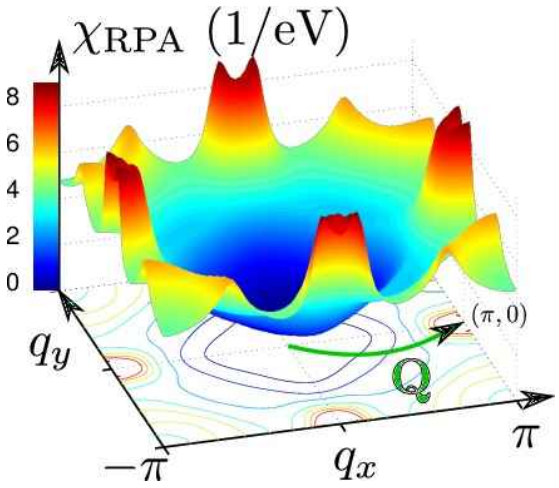




Superconductivity

- superconducting order parameter from spin- fluctuation theory

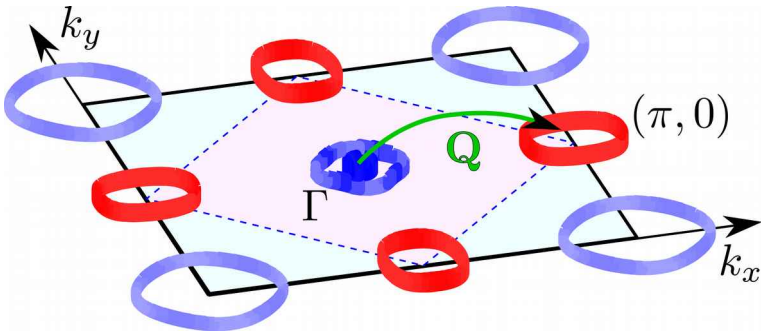
$$H_{\mathrm{BCS}} = -\sum_{\mathbf{R},\mathbf{R}'} \Delta_{\mathbf{R}\mathbf{R}'} c^{\dagger}_{\mathbf{R}\uparrow} c^{\dagger}_{\mathbf{R}'\downarrow} + H.c.,$$



- calculate Greens 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

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

$$H_{\mathrm{imp}} = \sum_{\sigma} V_{\mathrm{imp}} c^{\dagger}_{\mathbf{R}^*\sigma} c_{\mathbf{R}^*\sigma} \qquad H = H_0 + H_{\mathrm{BCS}} + H_{\mathrm{imp}}$$

- T-matrix approach to obtain Greens function

  other methods also possible
  - BdG
  - Gutzwiller mean field

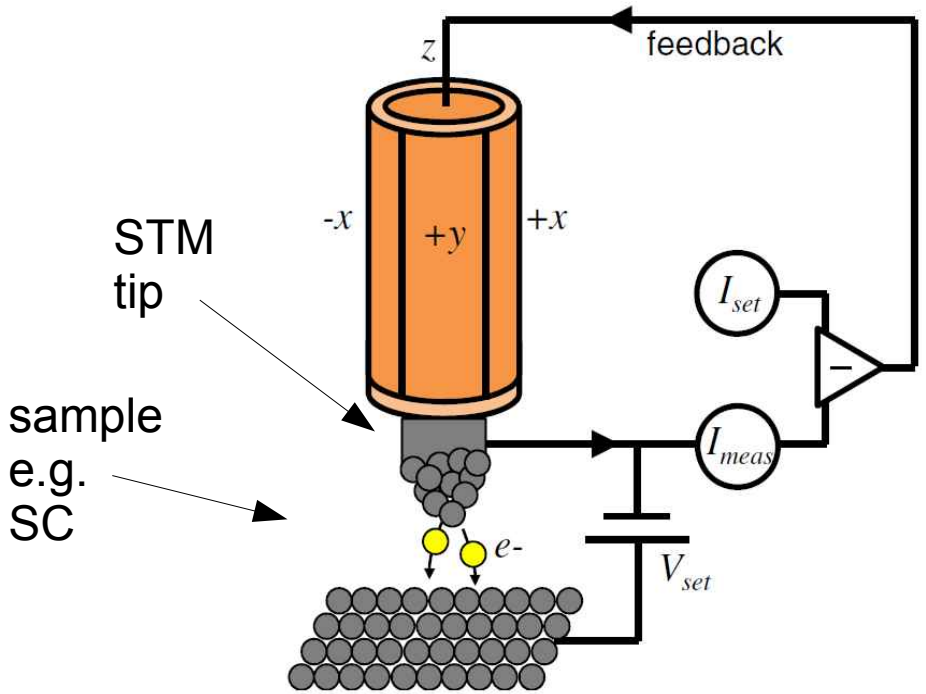
Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey et al., New J. Phys. **19**, 013028 (2017)

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

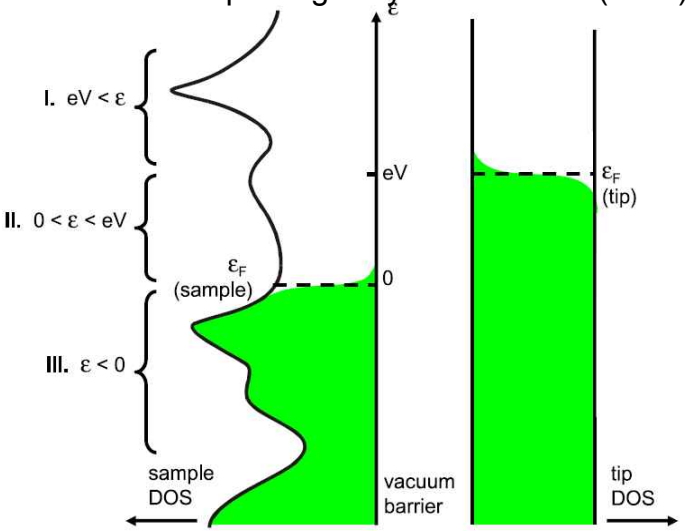
$$\underline{\hat{T}}(\omega) = [1 - \underline{\hat{V}}_{\mathrm{imp}}\underline{\hat{G}}(\omega)]^{-1}\underline{\hat{V}}_{\mathrm{imp}}$$

lattice Green function
(state of the art)

Scanning tunneling microscopy



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



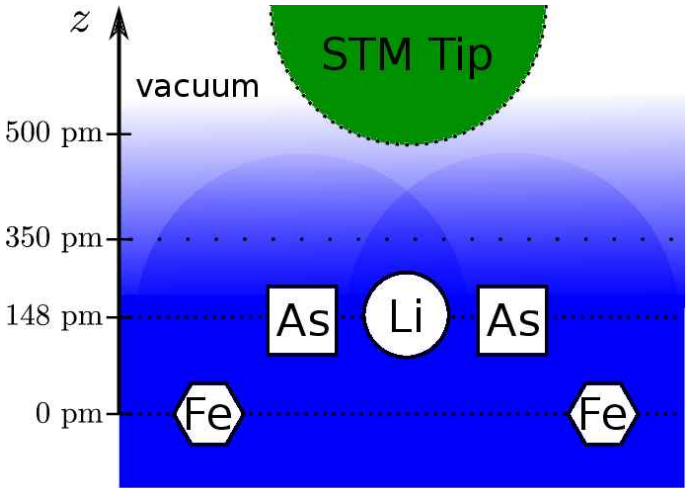
Tunnelling current:

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

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

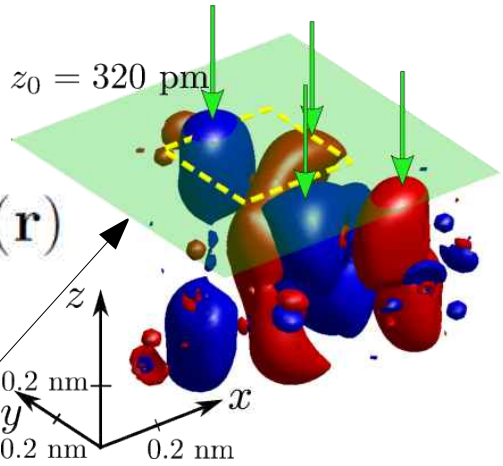
Local Density Of States (LDOS)
of sample at given energy at the tip position

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



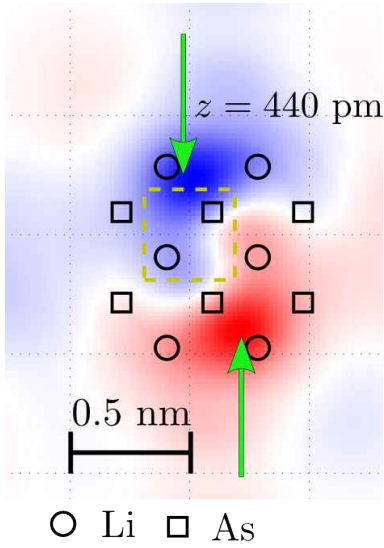
continuum LDOS (cLDOS)

- 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

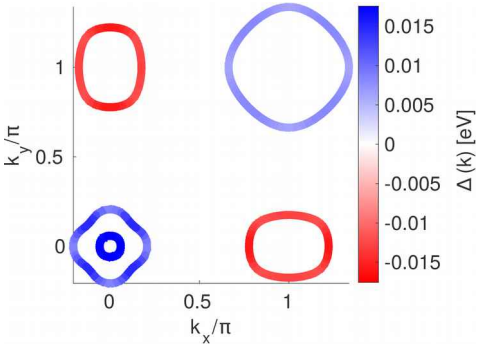
continuum Local Density Of States (cLDOS) of sample at given energy at the tip position

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

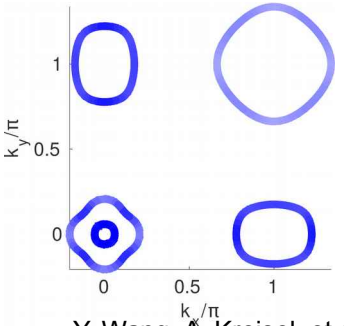
LiFeAs: Questions

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

conventional $s_{\pm}$

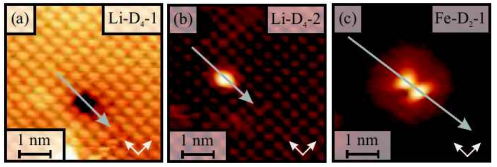


conventional s_{++}



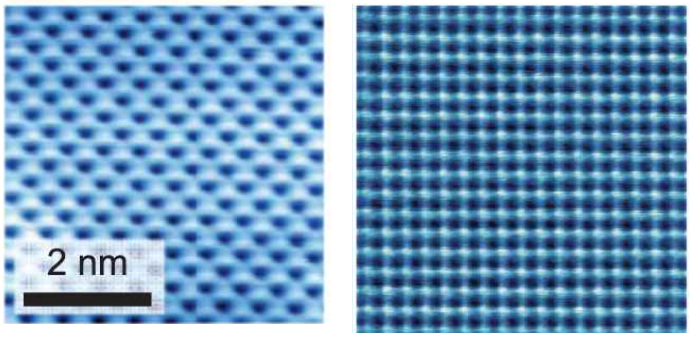
Y. Wang, A. Kreisel, et al. Phys. Rev. B **88**, 174516 (2013)
Z. P. Yin, K. Haule, G. Kotliar Nature Physics **10**, 845 (2014)
T. Saito, et al. Phys. Rev. B **90**, 035104 (2014)
F. Ahn, et al. Phys. Rev. B **89**, 144513 (2014)

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



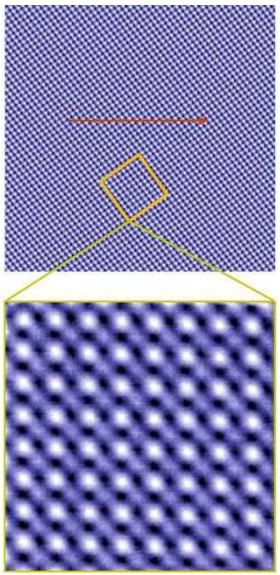
Hanaguri, unpublished (KITP 2011)

  - registered "surface lattice" in STM



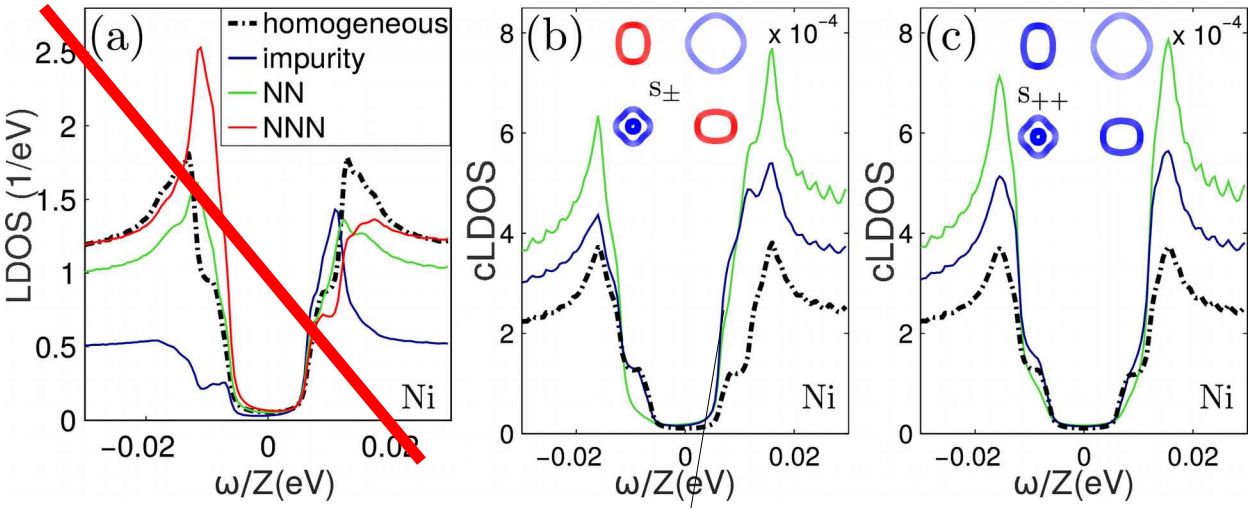
LiFeAs: Li or As lattice?

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)



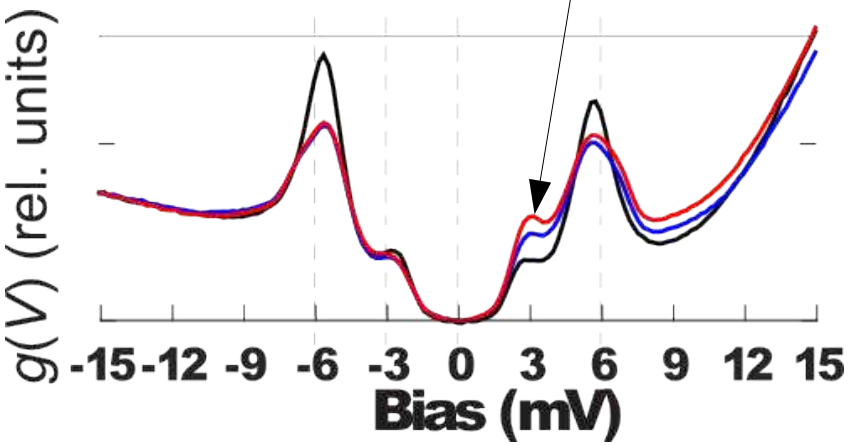
LiFeAs: spectra

- evidence for sign-changing order parameter by in-gap state with known impurity (Ni)



lattice LDOS: strong response at negative bias

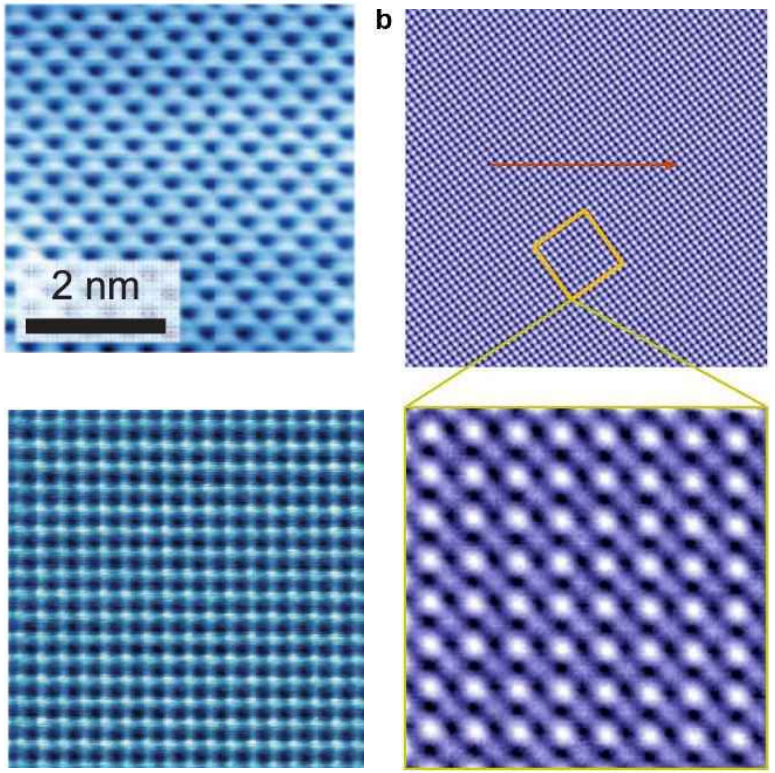
$$0 \approx 1 - V_{\mathrm{imp}}^{\mu\mu} G_{\mathbf{R}=0}^{0}(\omega)^{\mu\mu}$$



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

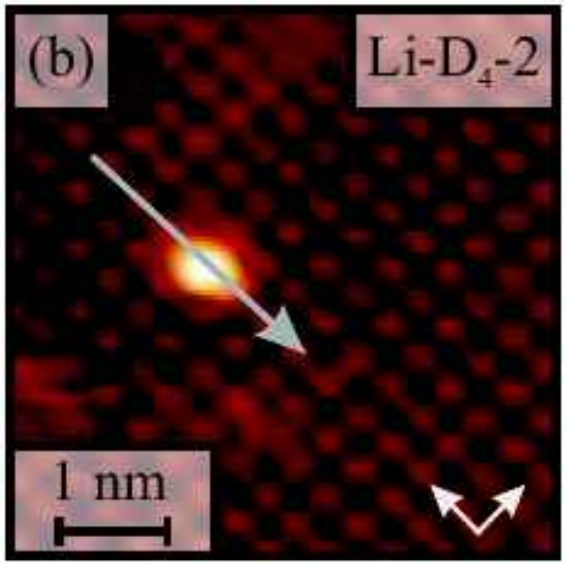
Height and current dependence of topographs

- 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



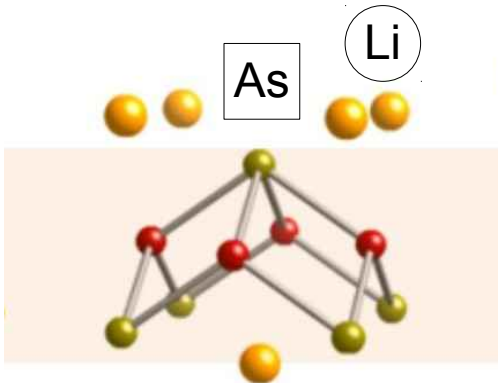
R. Schlegel, et al., Phys. Status Solidi B, **254**: 1600159 (2017)

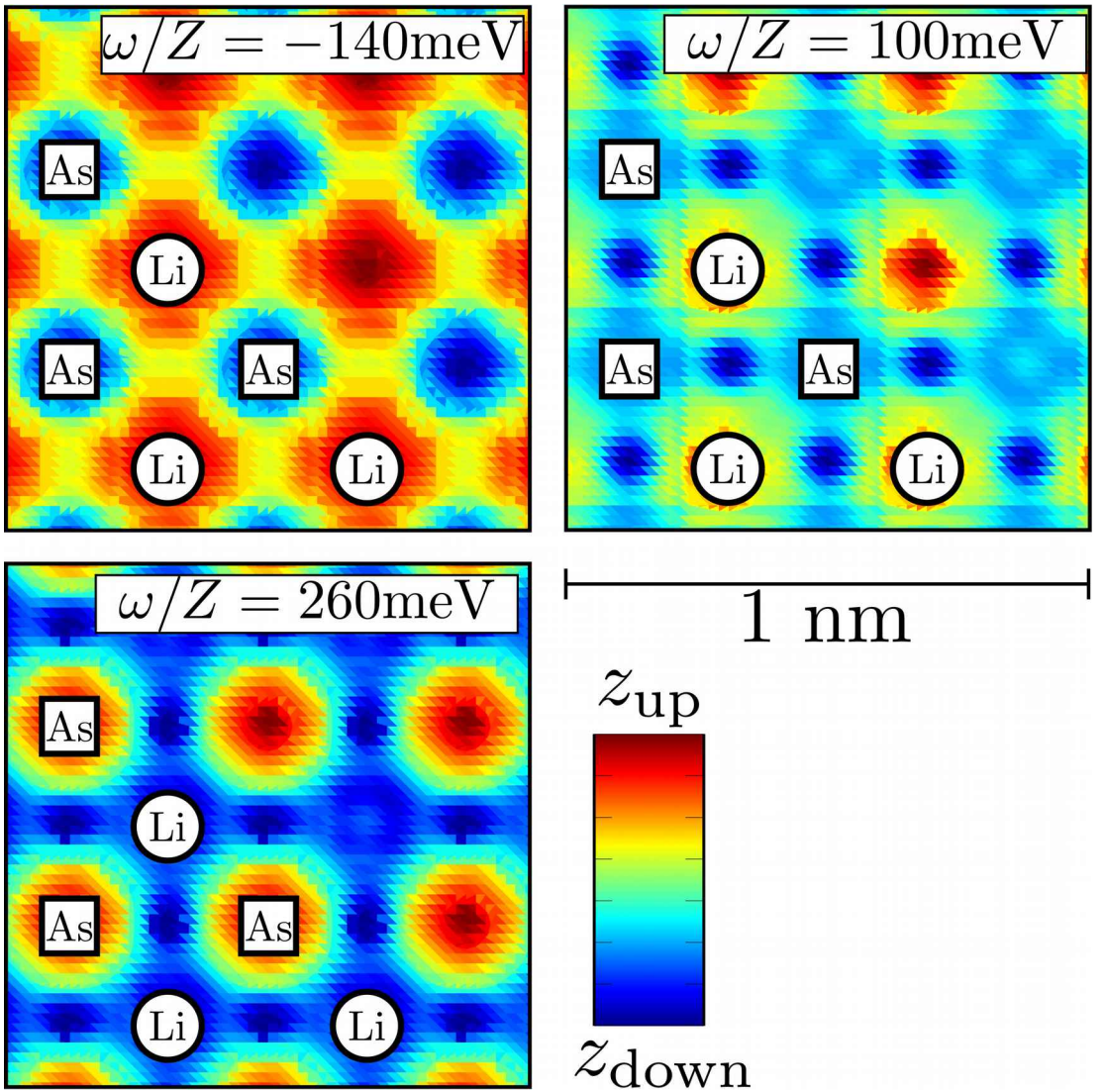
Simulation of topographs

- 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



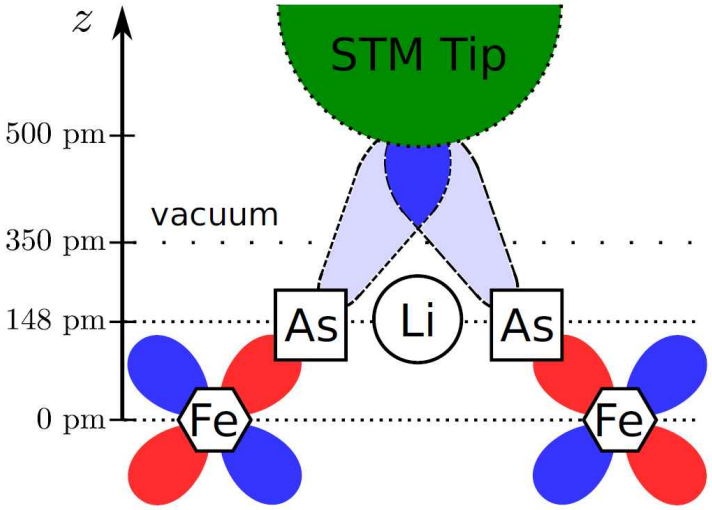


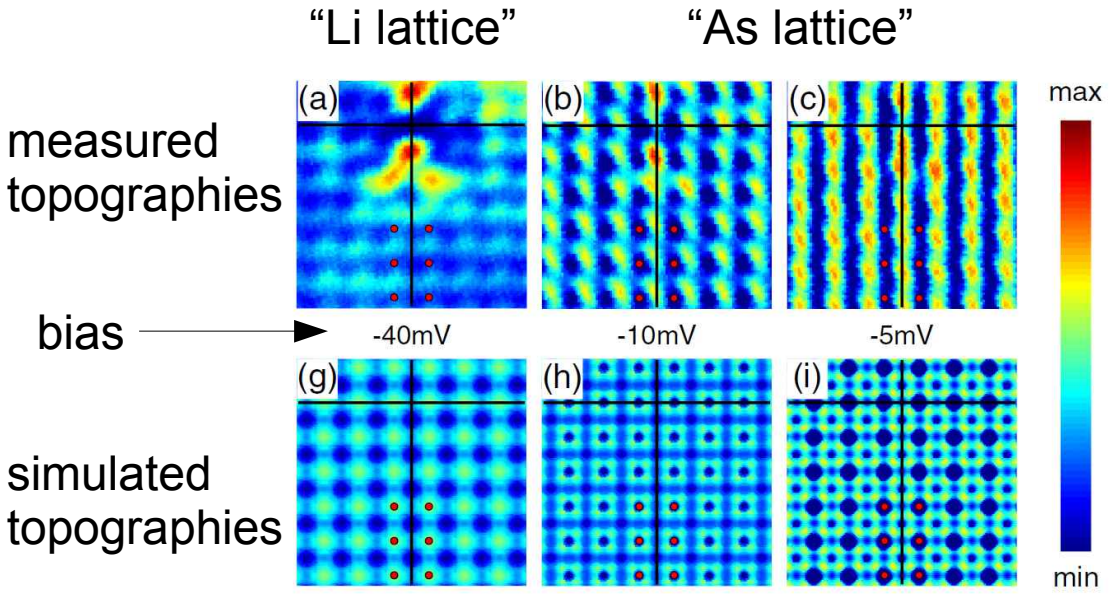
Results
registered surface lattice in STM

- 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

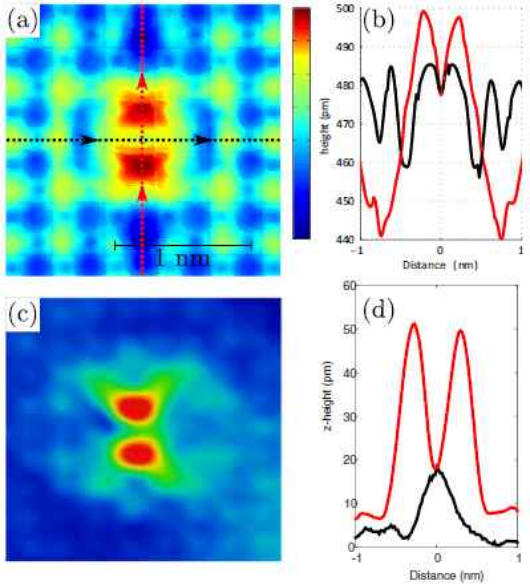




A. Kreisel, *et al.* Phys. Rev. B **94**, 224518 (2016)

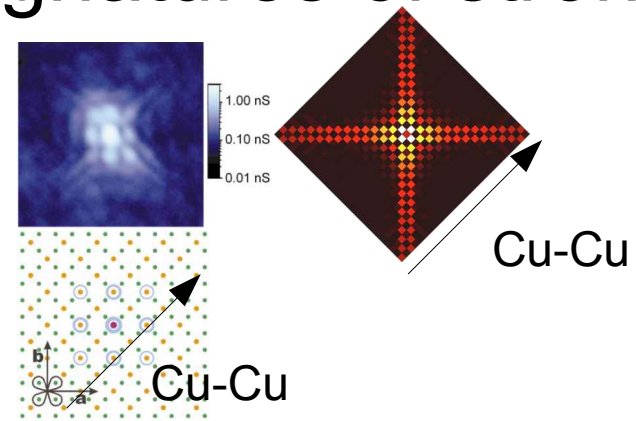
simulated topography close to strong imp.

measured topography close to Ni



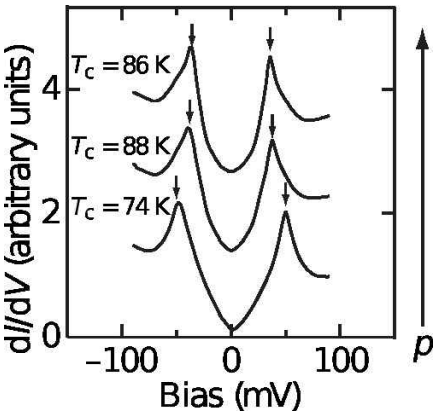
Cuprates: Questions

- signatures of strong impurity in d-wave SC

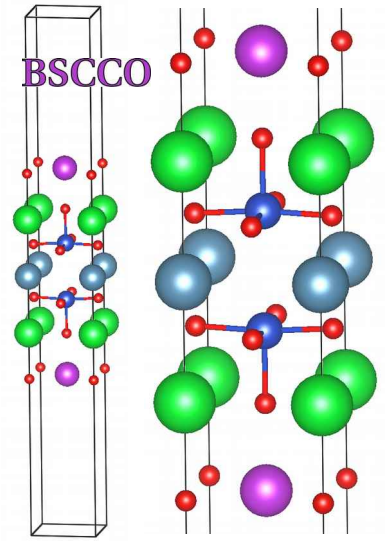


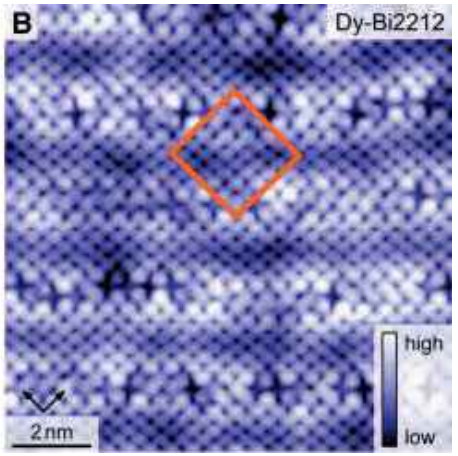
Kohsaka et al. Nature, **454**, 1072 (2008)

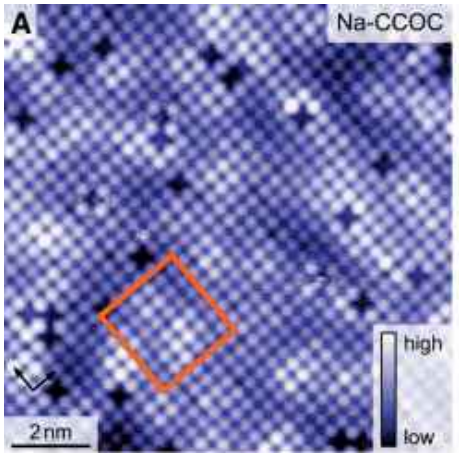
Crossover between U-shaped and V-shaped spectra

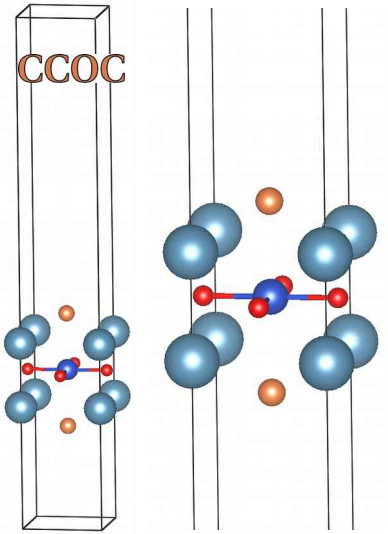


- universalities across materials





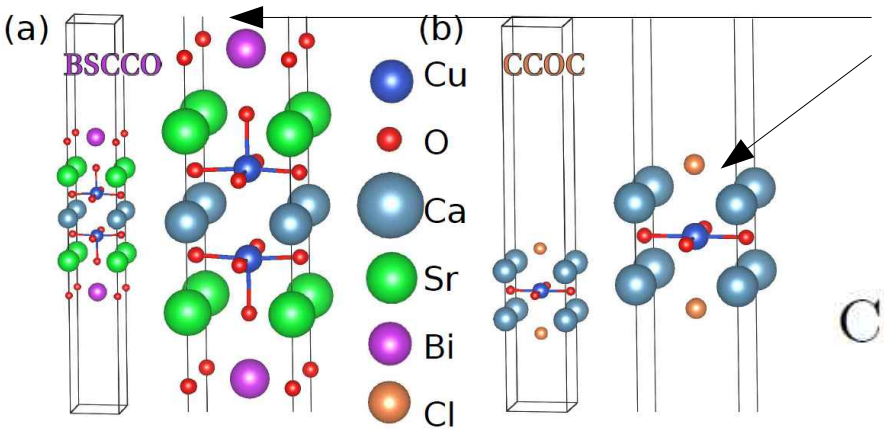




same properties for tunneling!

Wannier method: Cuprates

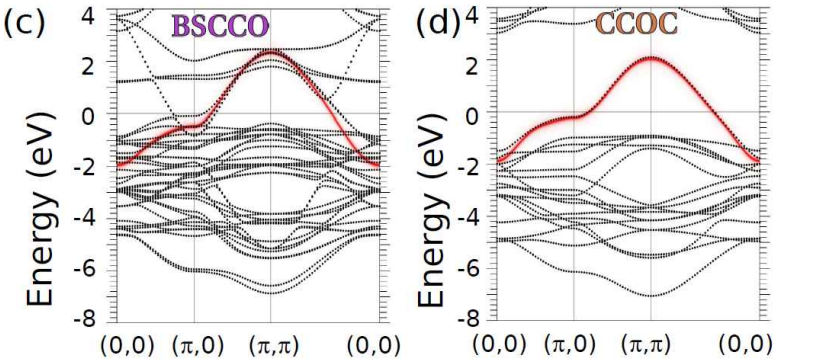
$Bi_2Sr_2CaCu_2O_8$

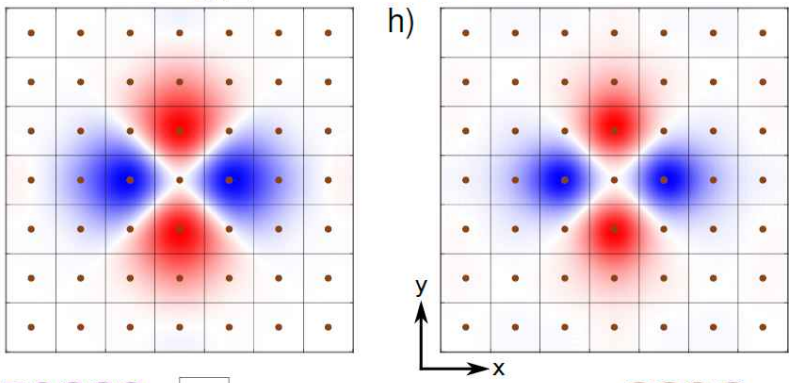


$Ca_2CuO_2Cl_2$

Surface
BiO vs. CaCl
and tunneling path
very different

Ab initio calculation:
1 band model
+Wanner function



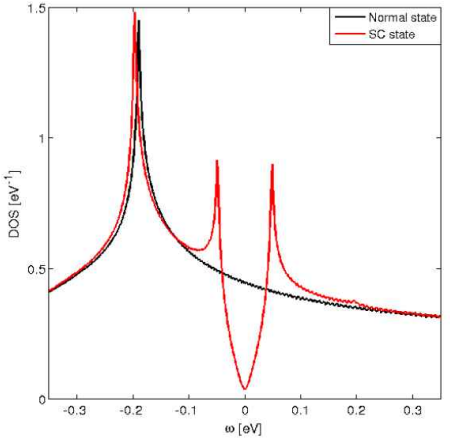


similar properties
dictated by
crystal symmetry

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

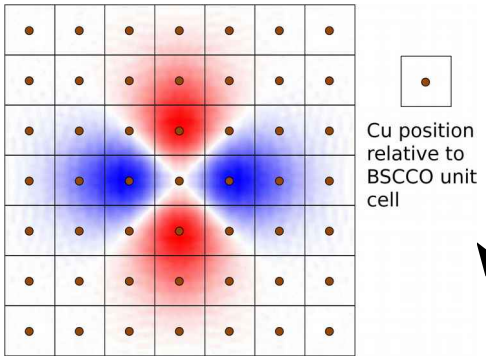
Superconductivity

- superconducting order parameter (d-wave) (phenomenology or calculation: 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

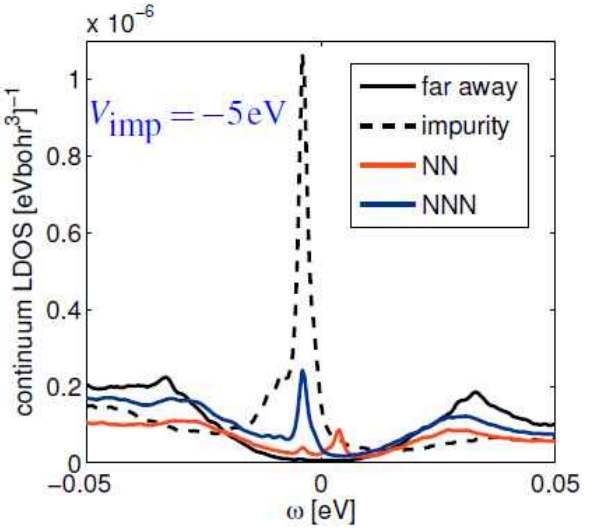
local density of states (LDOS)

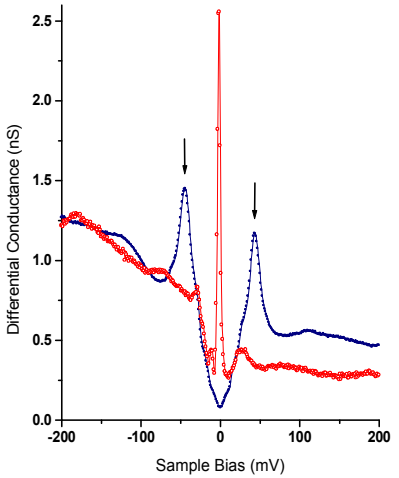
$$\rho(r,\omega) \equiv -\frac{1}{\pi} \operatorname{Im} G(\mathbf{r},\mathbf{r};\omega)$$

BSCCO: Results
STM maps and spectra

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

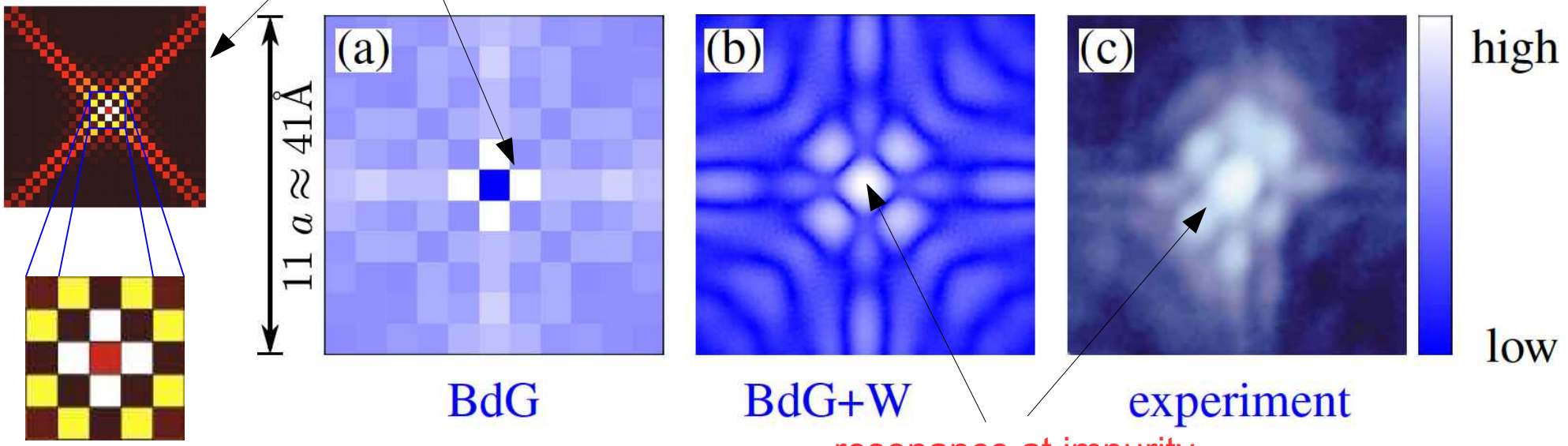
Pan et al., Nature **403**, 746 (2000)





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

resonance at NN

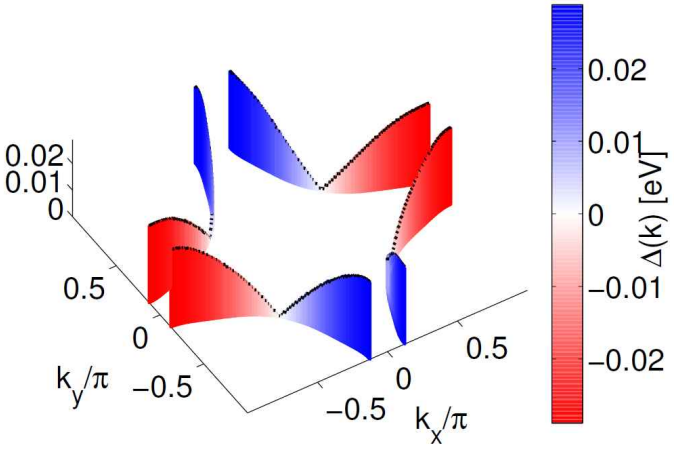


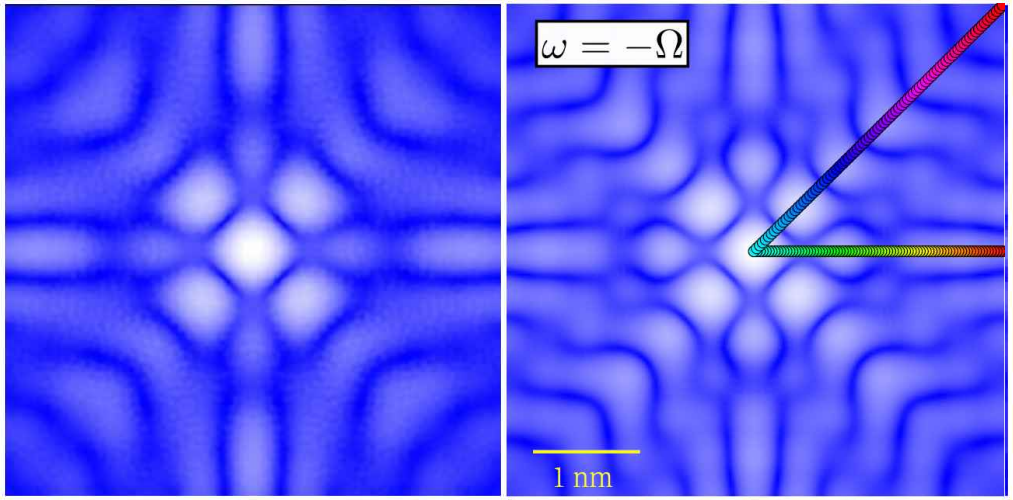
$Bi_2Sr_2CaCu_2O_8 \leftrightarrow Ca_2CuO_2Cl_2$

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

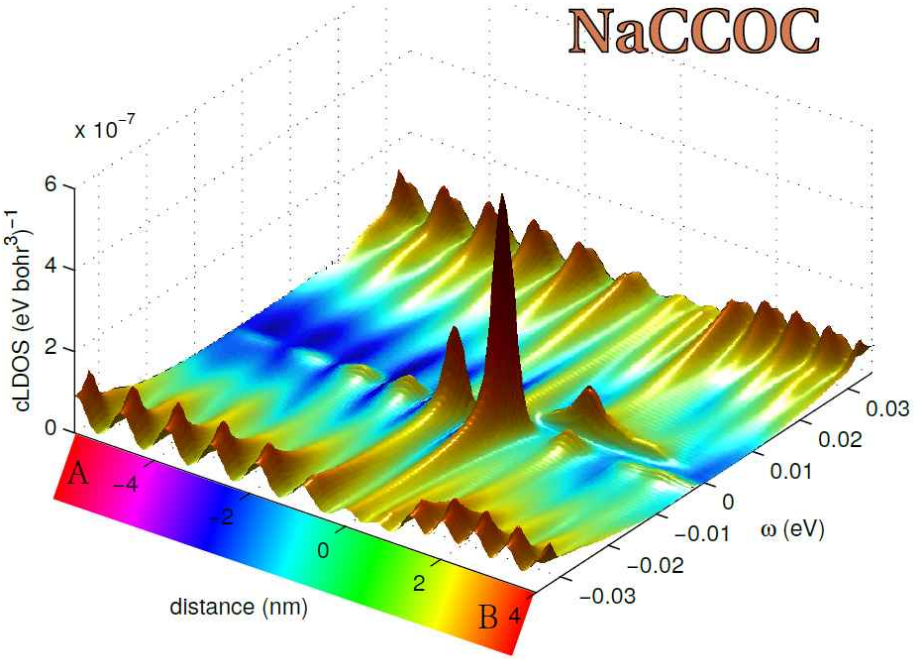
$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_{\mu,\nu,\mathbf{R},\mathbf{R}'} G(\mathbf{R},\mu,\mathbf{R}',\nu;\omega) w_{\mathbf{R},\mu}(\mathbf{r}) w^*_{\mathbf{R}',\nu}(\mathbf{r}')$$

- strong impurity
  spectra + conductance map





$Bi_2Sr_2CaCu_2O_8$ $Ca_2CuO_2Cl_2$

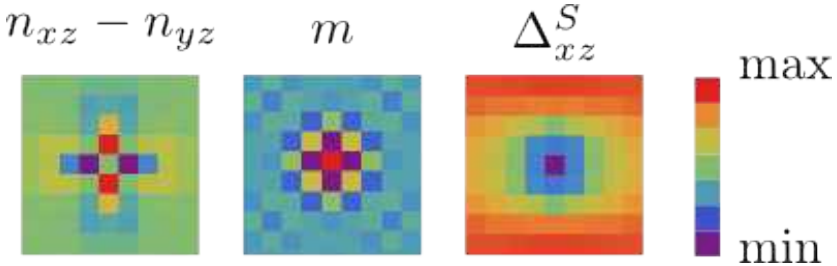


Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey et al., New J. Phys. **19**, 013028 (2017)
P. Choubey, *et al.*. Phys. Rev. B **96**, 174523 (2017)

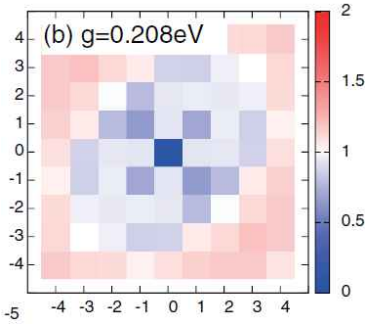
Chiral defects

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

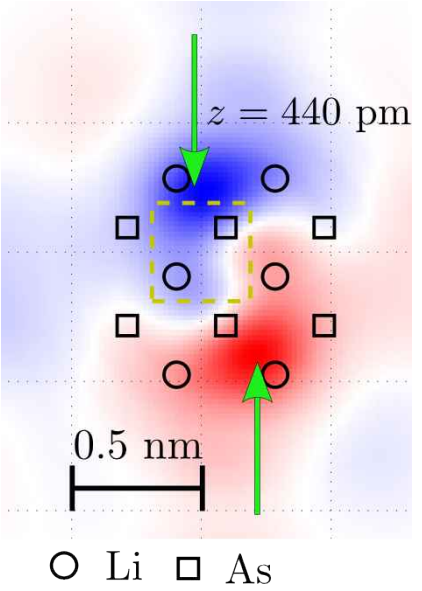
local orbital order
+ Wannier function
→ chiral defect structure



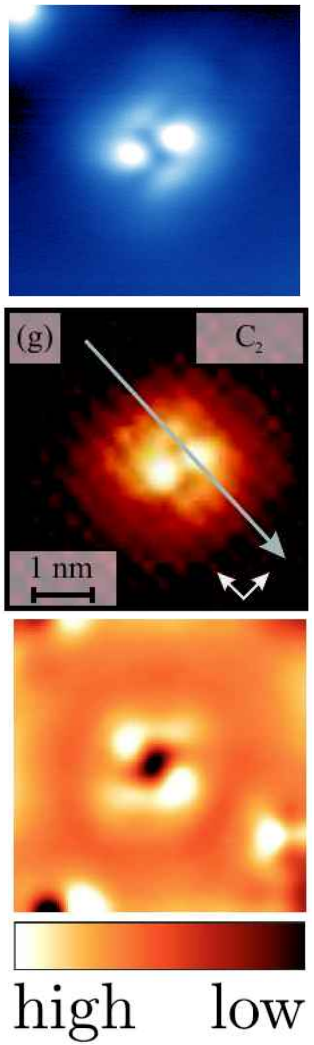
Gastiasoro, Andersen, J. Supercond Nov. Magn., **26**, 2651 (2013)



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

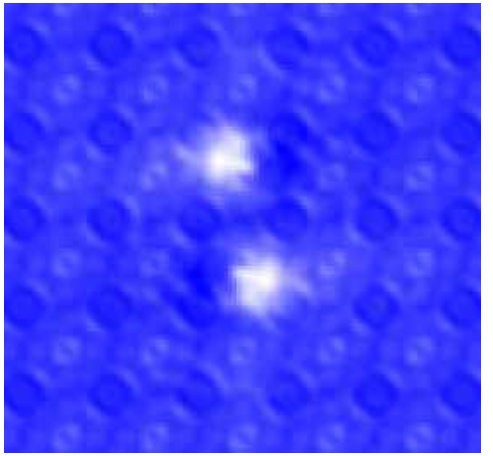


d_xz Wannier function on Fe(2)



FeSe: orbital selective electronic structure

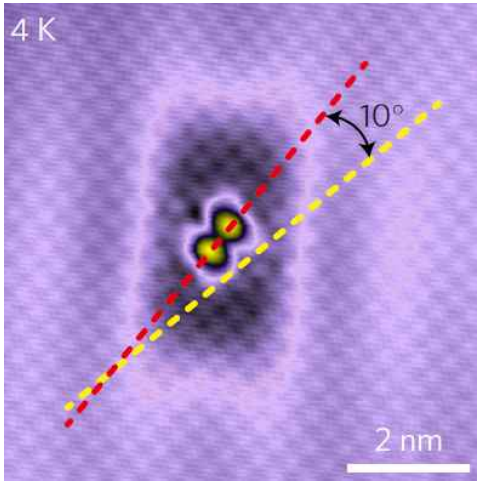
- Imprints on impurity states
  - Point-like impurity in electronic structure with nematic order
  - Strongly directed quasiparticle scattering via reduced coherence



- Use Green's function in conjunction with Wannier transformation

$$\tilde{G}_{\ell\ell'}(\mathbf{k},\omega_n) = \sqrt{Z_\ell Z_{\ell'}} \sum_\mu \frac{a_\mu^\ell(\mathbf{k}) a_\mu^{\ell'*}(\mathbf{k})}{i\omega_n - \tilde{E}_\mu(\mathbf{k})}$$

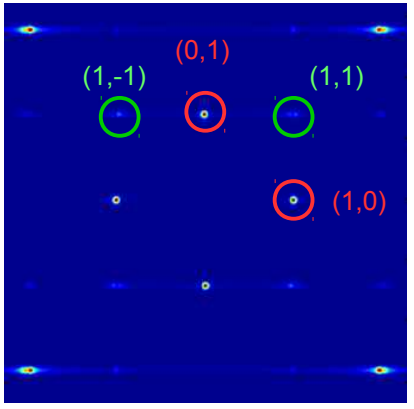
$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_{\mu,\nu,\mathbf{R},\mathbf{R}'} G(\mathbf{R},\mu,\mathbf{R}',\nu;\omega) w_{\mathbf{R},\mu}(\mathbf{r}) w^*_{\mathbf{R}',\nu}(\mathbf{r}')$$



Li et al., Nature Physics volume **13**, pages 957 (2017)

Imprints on cLDOS of homogeneous system

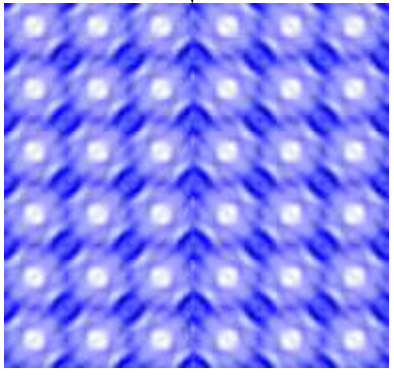
- Intra-unit cell information

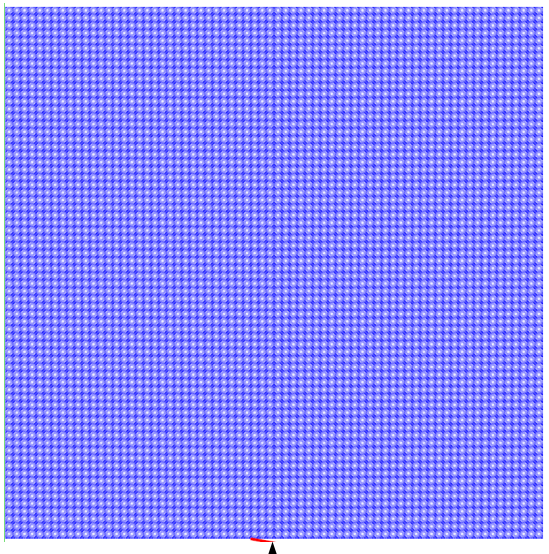


Mask (1,1) and (1,-1)
Fourier transform back, take difference

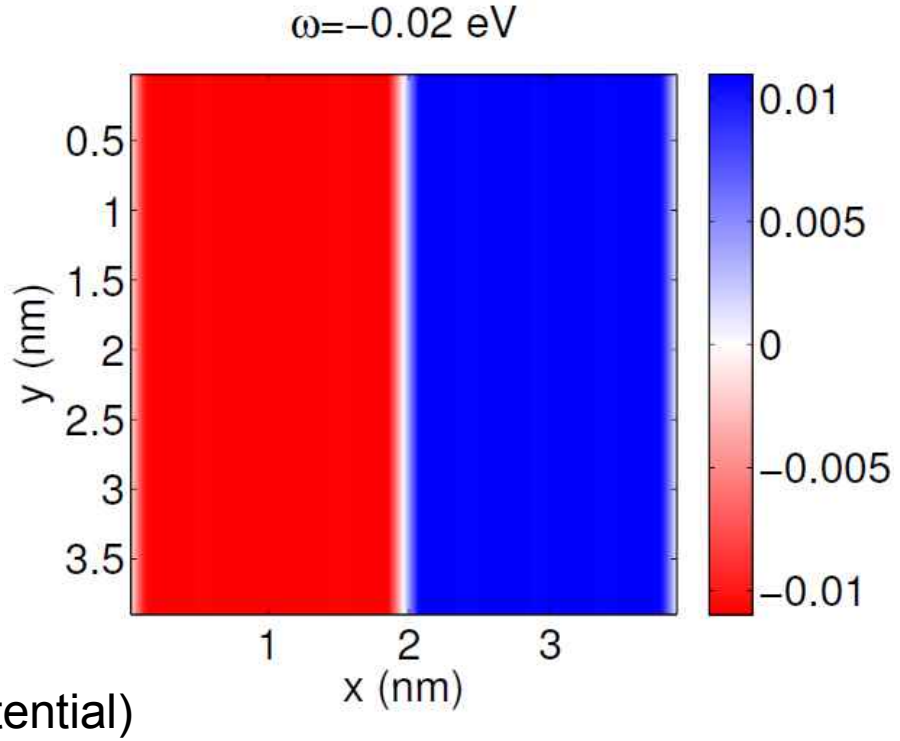
Fourier transform

Blow-up: Twin-boundary





Twin-boundary (no scattering potential)



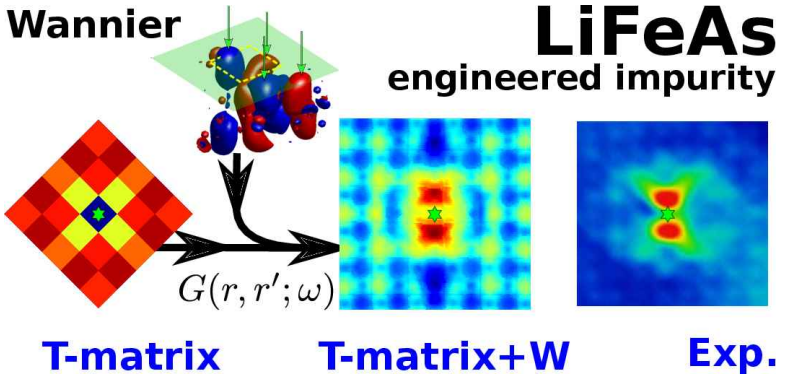
Summary

- Wannier method: basis transformation of the lattice Green function
- Qualitative correct (symmetry) and quantitative predictive results
- Impurities and homogeneous lattice in LiFeAs
- Universality in cuprates

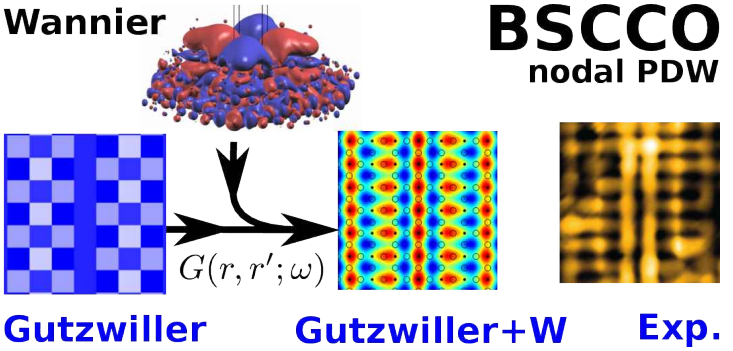
Kreisel et al., Phys. Rev. Lett. **114**, 217002 (2015)
Choubey, *et al.*. Phys. Rev. B **96**, 174523 (2017)

- Nematicity in Fe-based SC

Sprau, et al. Science, **357**, 75 (2017)
A. Kostin,et al., arXiv:1802.02266

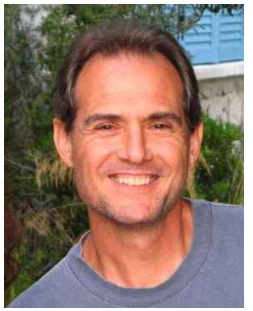


S. Chi, (...) , **A. Kreisel**, *et al.* Phys. Rev. B **94**, 134515 (2016)
A. Kreisel, *et al.* Phys. Rev. B **94**, 224518 (2016)



Choubey et al., New J. Phys. **19**, 013028 (2017)

Acknowledgments

Tight binding models and Wannier functions available
www.physik.uni-leipzig.de/~kreisel/model.php