Towards a quantitative description of tunneling conductance of superconductors

Andreas Kreisel

Institut für Theoretische Physik, Universität Leipzig, Germany

R. Nelson
RWTH Aachen University, Germany

T. Berlijn
CNMS, Oak Ridge Nat. Lab., USA

W. Ku
Dept. of Phys. and Astr., Shanghai Jiao Tong U., China

S. Chi, R. Liang, W.N. Hardy, D.A. Bonn
Dept. of Phys. and Astr., UBC, Canada

R. Aluru, P. Wahl, H. Zhou
SUPA, U. St. Andrews, UK

U.R. Singh
MPI-FKF, Stuttgart, Germany

P.J. Hirschfeld
Dept. of Physics, U. Florida, USA

B.M. Andersen
Niels Bohr Institute, U. Copenhagen, Denmark

UNIVERSITÄT LEIPZIG

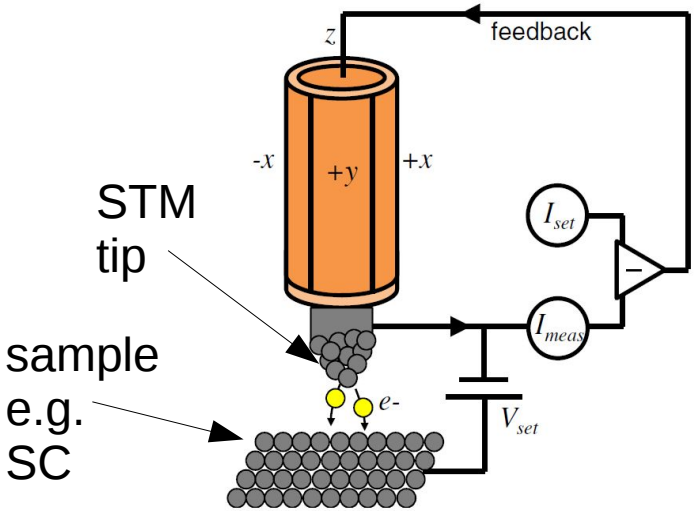
UF UNIVERSITY of FLORIDA
The Foundation for The Gator Nation

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

Experiment: R. Aluru: C39.00005: Impact of iron-site defects on superconductivity in LiFeAs
3:18 PM–3:30 PM

KØBENHAVNS UNIVERSITET

Scanning tunneling microscopy

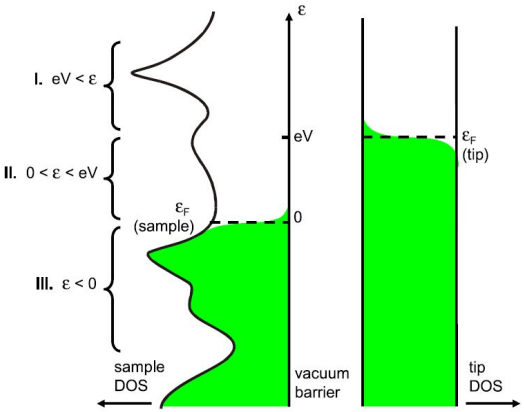


J. Hoffman 2011 Rep. Prog. Phys. **74** 124513 (2011)

Tunneling current:

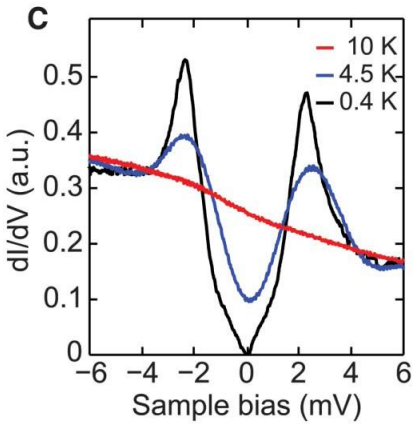
$$I(V,x,y,z) = -\frac{4\pi e}{\hbar}\rho_t(0)|M|^2 \int_0^{eV} \rho(x,y,z,\epsilon)d\epsilon$$

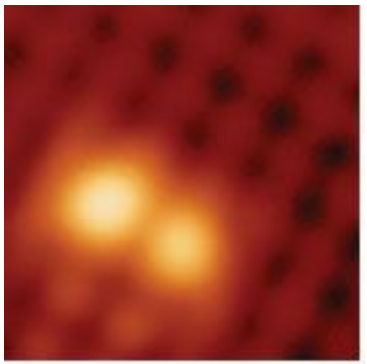
Local Density Of States (LDOS)
of sample at tip position



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

FeSe: STM spectra
topograph of Fe centered impurity

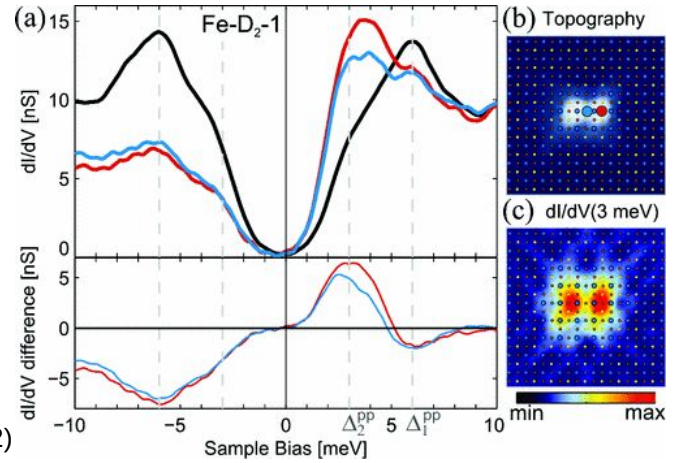




Song et al., Science **332**, 1410 (2011)

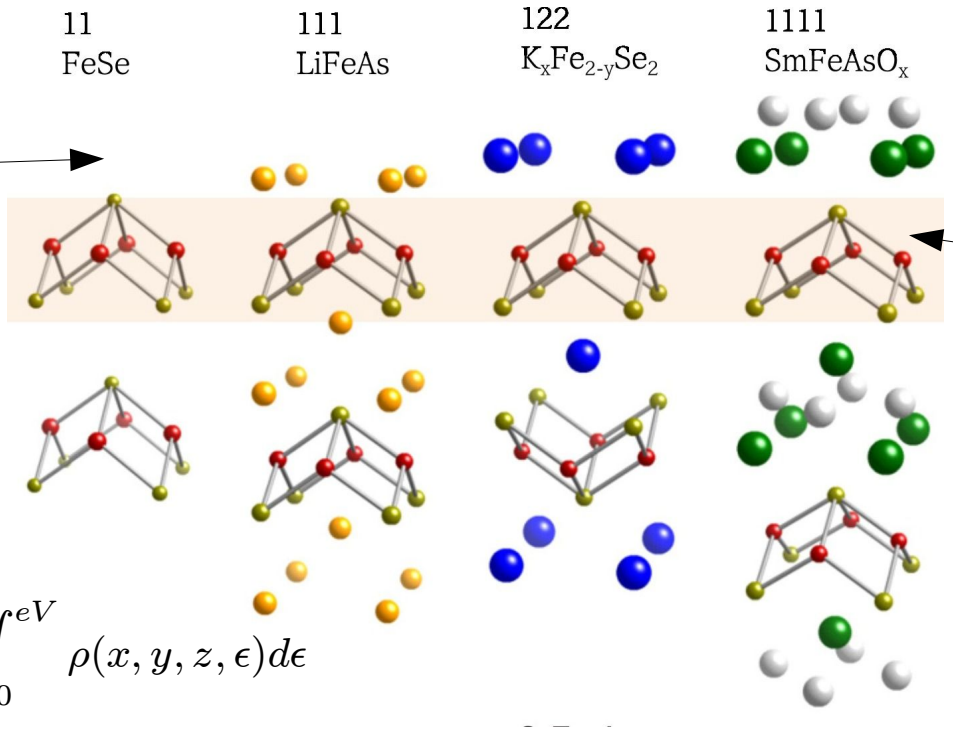
Can-Li Song, et al. PRL **109**, 137004 (2012)

LiFeAs: STM spectra
topograph of Fe centered impurity



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

Fe-SC: layered superconductors



surface termination:
Se (FeSe)
Li (LiFeAs)

common layer:
states at the
Fermi level

LDOS of sample at given energy at the tip position

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

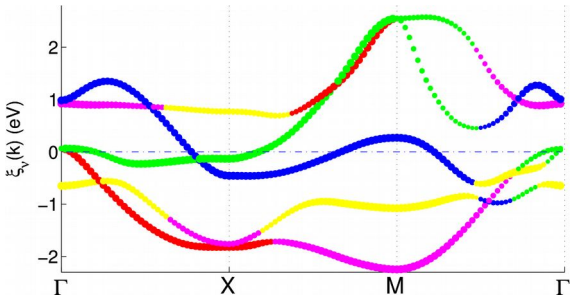
- Theories
  - "Filter function": STM tip probes states in the superconducting layer by tunneling matrix elements (Cuprates) Martin *et al.*, PRL **88**, 097003 (2002)
  - Large tight binding basis set of orbitals + Green function method to calculate tunneling matrix elements J. Nieminen, *et al.,* PRB **80**, 134509 (2009)
  - Wannier method: take into account surface wavefunction as obtained from ab-initio methods Choubey et al., PRB **90**, 134520 (2014)
    Kreisel et al., PRL **114**, 217002 (2015)

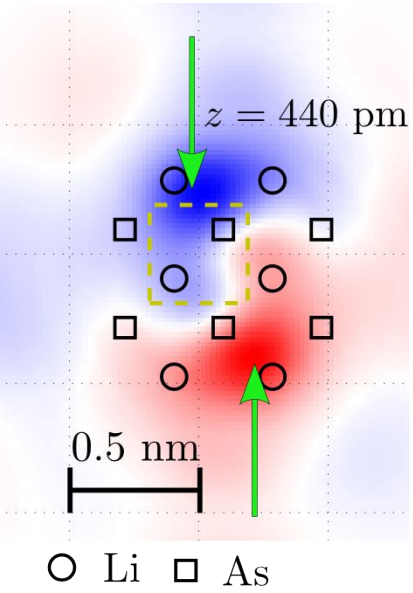
Example: LiFeAs

- pristine superconductor (few impurities)
- non-polar surface (excellent to study via STM)

- Ab-initio calculations
  - band structure

    5 band model
  - Wannier functions (including glide plane symmetry)

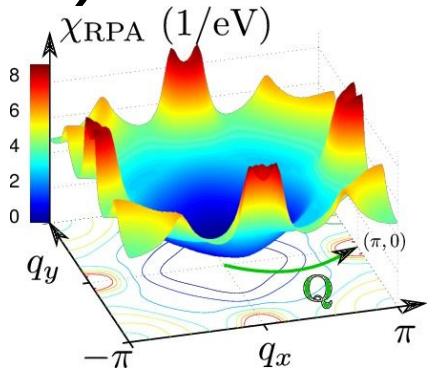


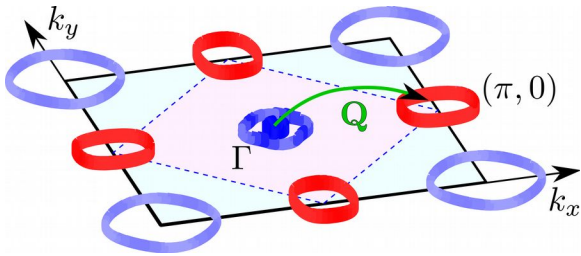


  - known impurities: calculation of impurity potential for Ni, Mn, Co

Theory: Wannier method

- Input from ab-initio calculation (bands, impurity potential)
- superconducting order parameter from spin-fluctuation theory





- impurity via T-matrix calculation

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

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

lattice Green function (state of the art)

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

Basis transformation to continuum Green function (Wannier method)

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

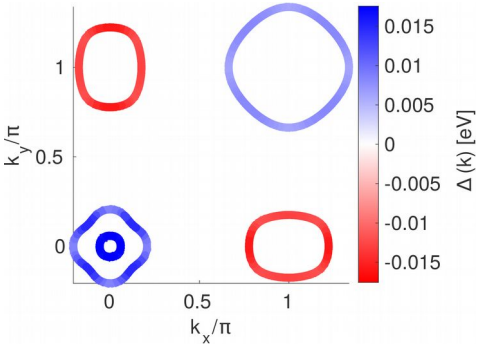
continuum local density of states (cLDOS) at the tip position

Questions

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

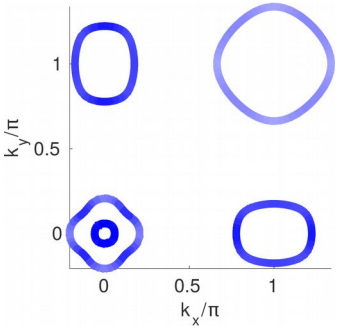
conventional $s_{\pm}$

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

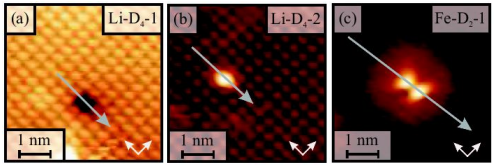


conventional s_{++}

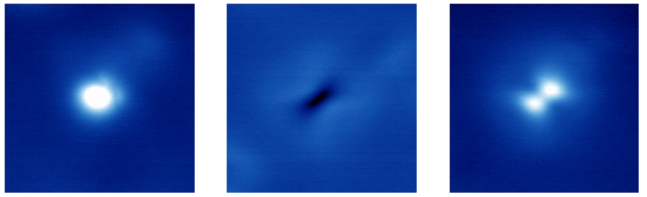
Tetsuro Saito, et al.
Phys. Rev. B 90, 035104 (2014)



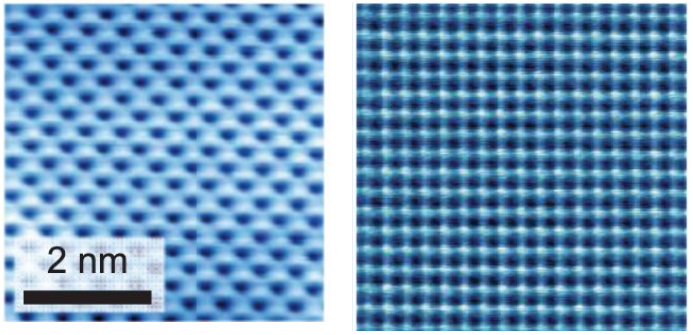
R. Schlegel, et al., Phys. Status Solidi B, **254**: 1600159 (2017)

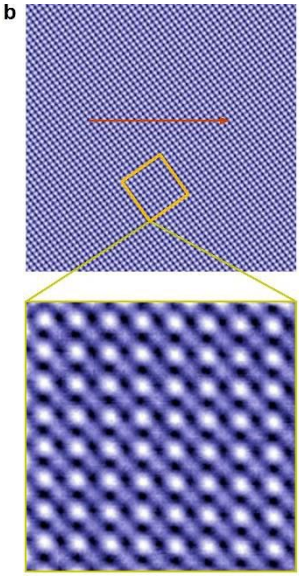


Hanaguri, unpublished (KITP 2011)



  - registered “surface lattice” in STM



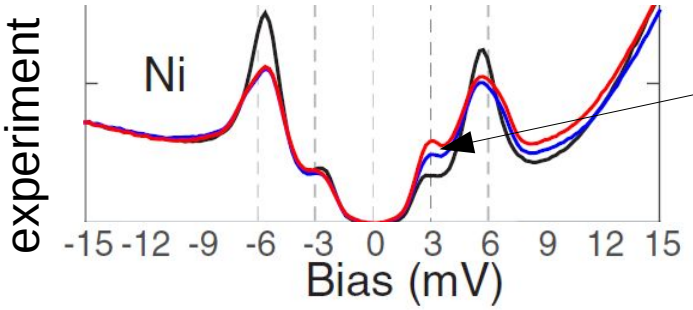


LiFeAs: Li or As lattice?

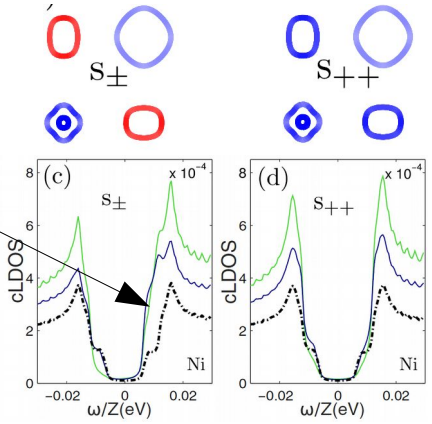
Shun Chi, et al., PRL 109, 087002 (2012)
T. Hanaguri, et al. PRB 85, 214505 (2012)
S. Grothe, et al., PRB 86, 174503 (2012)
J. -X. Yin, et al., arXiv, 1602.04949 (2016)

Results
order parameter ↔ impurities

- Requirement of s_{+-} state for bound states at lower gap edge

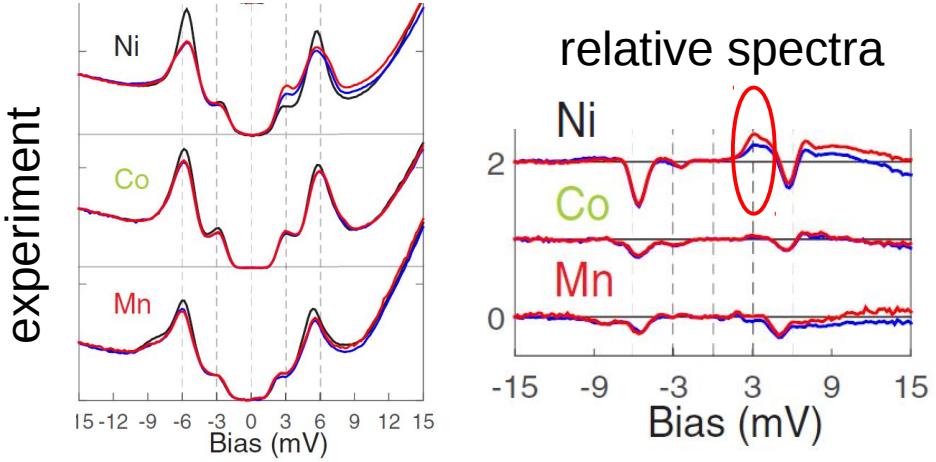


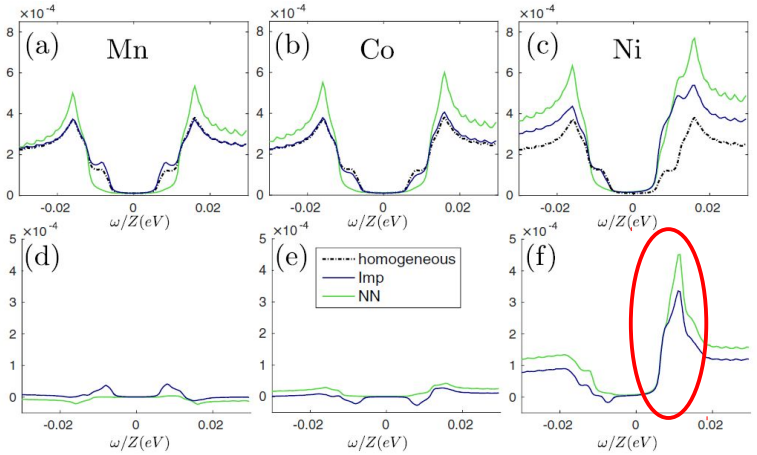
$$0 \approx 1 - V_{\mathrm{imp}}^{\mu\mu} G_{\mathbf{R}=0}^{0}(\omega)^{\mu\mu}$$



Talk: Ram Aluru C39.00005

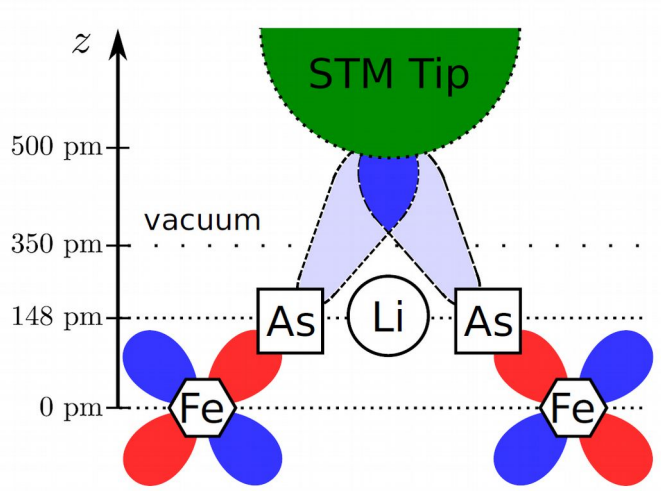
- sequence of calculated impurity potentials in agreement with experimental findings for engineered impurities

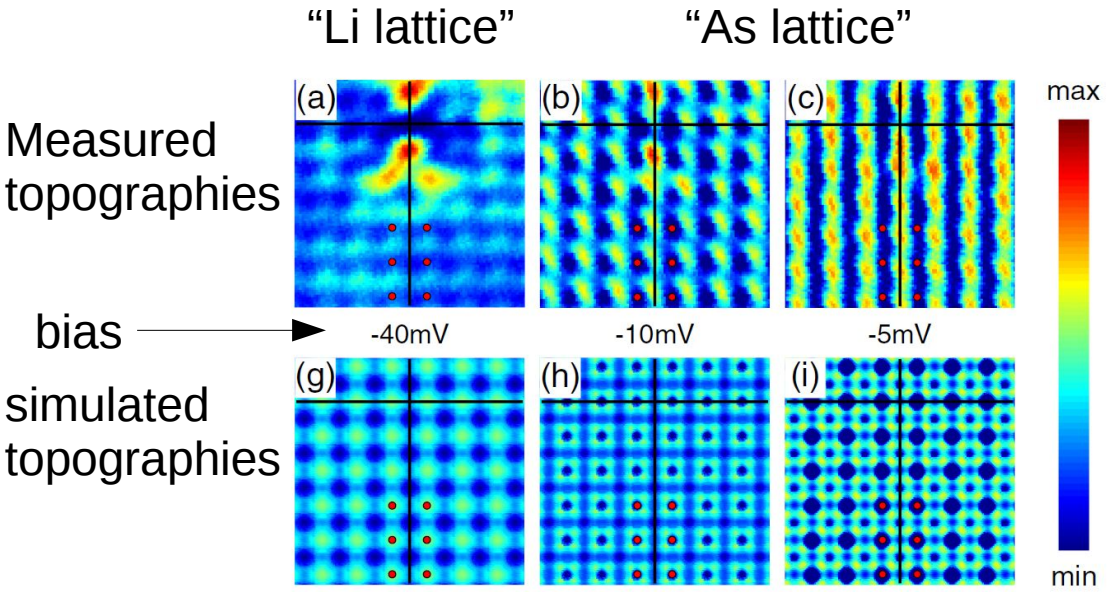




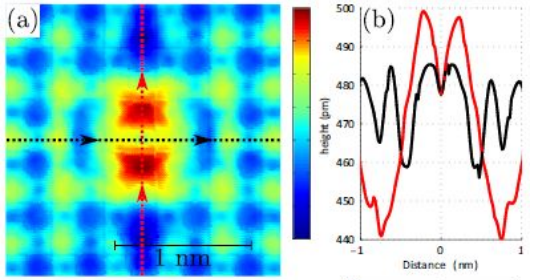
Results
registered surface lattice in STM

- Tunneling into states described by Wannier functions
- Registered lattice switches as function of bias and current

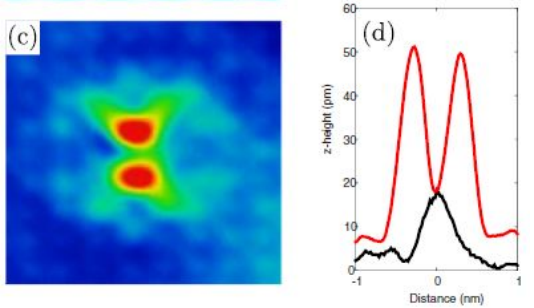




simulated topography close to strong imp.

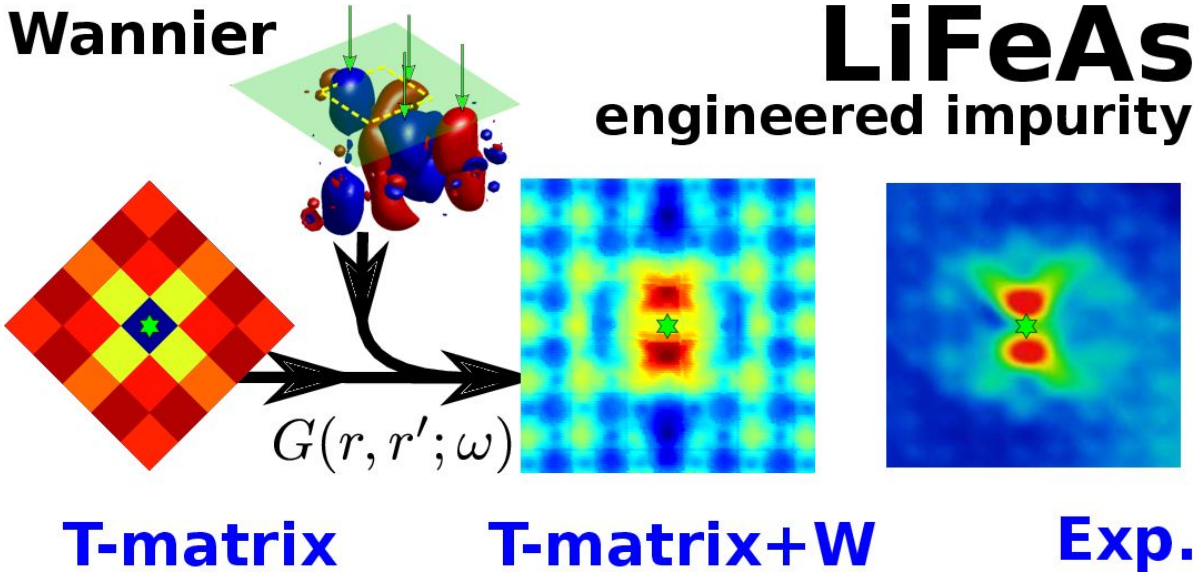


Measured topography close to Ni



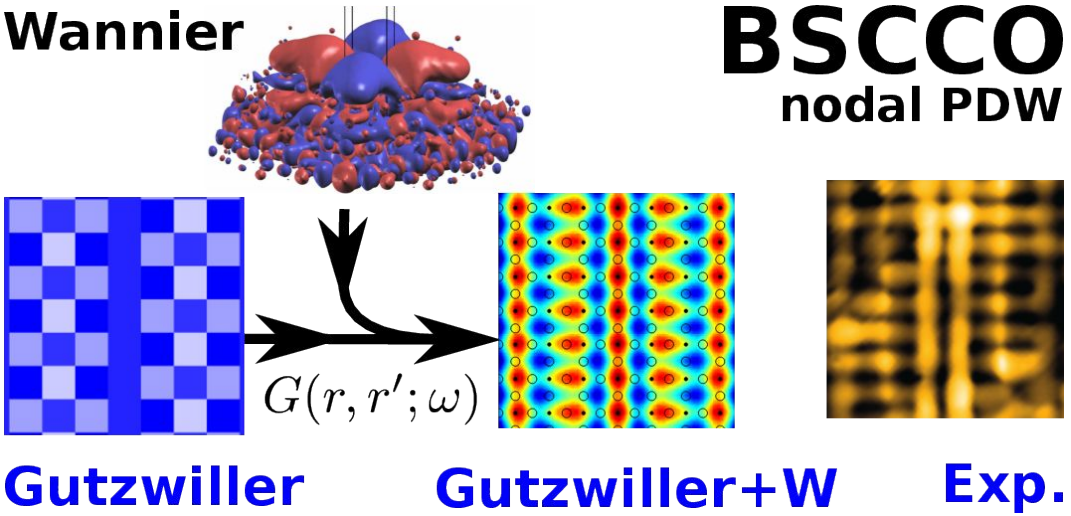
Summary

Talk: Ram Aluru
C39.00005 : Impact of iron-site defects on superconductivity in LiFeAs 3:18 PM–3:30 PM



- good description of “engineered” impurity properties (ab-initio potential, real space properties, bound states at lower gap edge)
- Switching of registered lattice depending on tip height and setpoint bias

Talk: P. Choubey Thursday, March 16, 2017 S41.00004 11:51 AM–12:03 PM



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

Acknowledgments