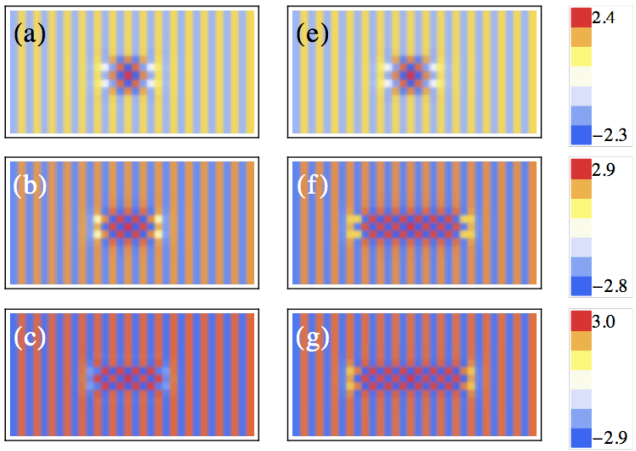
*Recent developments in Fe-based high-temperature superconductors*

New York 2013

# Disorder and nematicitity in Fe-based superconductors

Brian Møller Andersen

Niels Bohr Institute, University of Copenhagen



# Collaborators

Maria Navarro Gastiasoro

Astrid T. Rømer

Peter J. Hirschfeld

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Maria N. Gastiasoro

Astrid T. Rømer

Peter J. Hirschfeld

**Realistic five-band modelling of sub-gap impurity states in iron-based superconductors**

Maria N. Gastiasoro[1], P. J. Hirschfeld[2], and Brian M. Andersen[1]
[1] *Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark*
[2] *Department of Physics, University of Florida, Gainesville, Florida 32611, USA*
(Dated: September 4, 2013)

M. Gastiasoro *et al*, *preprint*

**Origin of electronic dimers in the spin-density wave phase of Fe-based superconductors**

Maria N. Gastiasoro[1], P. J. Hirschfeld[2], and Brian M. Andersen[1]
[1] *Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark*
[2] *Department of Physics, University of Florida, Gainesville, Florida 32611, USA*
(Dated: July 19, 2013)

M. Gastiasoro *et al*, 1307.4913

# Outline

1a) Overview of selected experimental data (STM)

1b)Theoretical modeling:
- SC phase (realistic modeling of bound states)

2a) Overview of selected experimental data (STM, transport)

2b)Theoretical modeling:
- SDW phase (emergent impurity states, anisotropic scatterers)

3) Conclusions

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# The disorder probe: local effects

Cuprates: Impurity states → d-wave symmetry.

**Interplay of magnetism and high-$T_c$ superconductivity at individual Ni impurity atoms in $Bi_2Sr_2CaCu_2O_{8+\delta}$**

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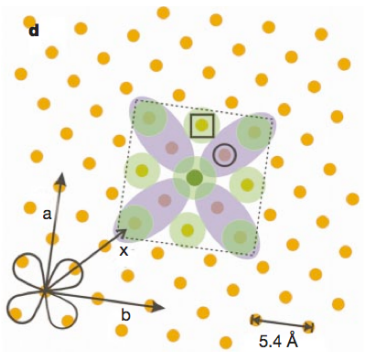


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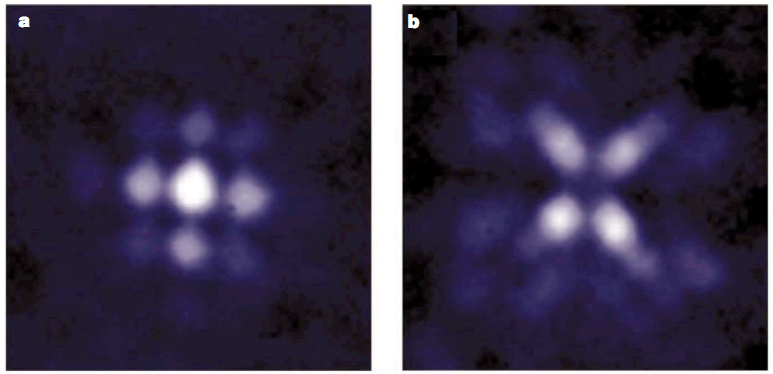

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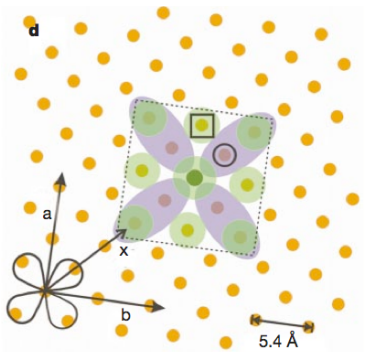


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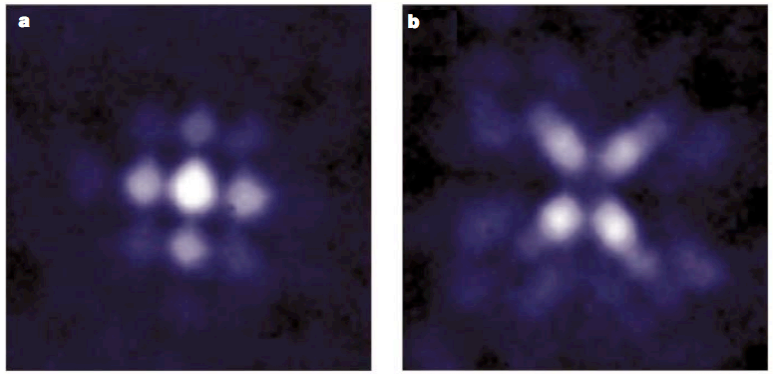
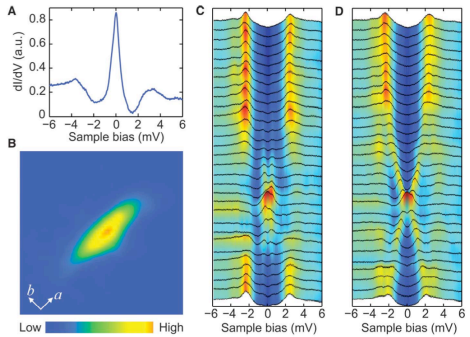
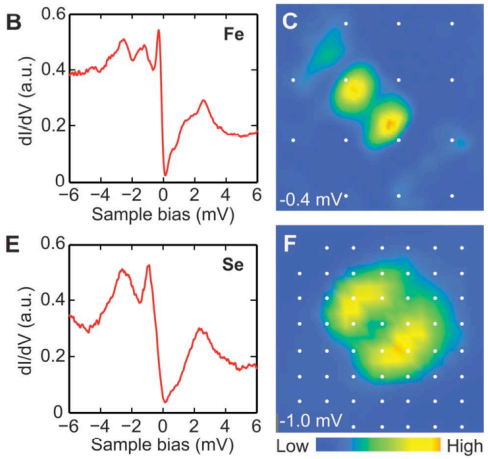



Pnictides: What can similar experiments reveal about the properties of the ground state?

# Direct Observation of Nodes and Twofold Symmetry in FeSe Superconductor

Can-Li Song,[1,2] Yi-Lin Wang,[2] Peng Cheng,[1] Ye-Ping Jiang,[1,2] Wei Li,[1] Tong Zhang,[1,2] Zhi Li,[2] Ke He,[2] Lili Wang,[2] Jin-Feng Jia,[1] Hsiang-Hsuan Hung,[3] Congjun Wu,[3] Xucun Ma,[2*] Xi Chen,[1*] Qi-Kun Xue[1,2]

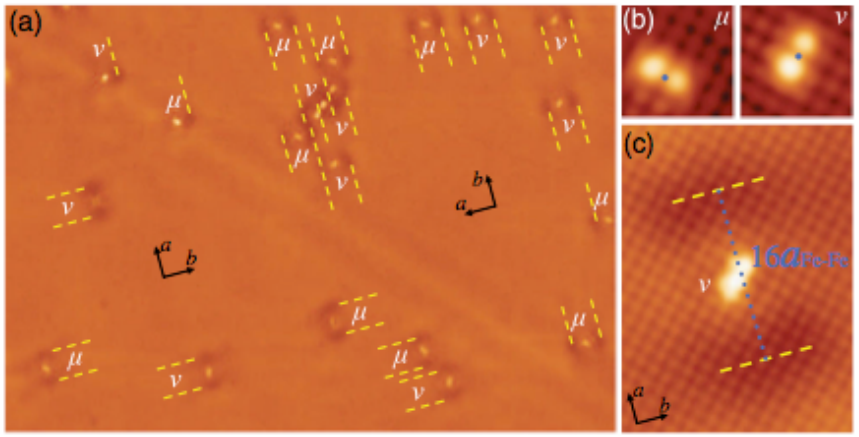



PRL 109, 137004 (2012) PHYSICAL REVIEW LETTERS week ending 28 SEPTEMBER 2012

## Suppression of Superconductivity by Twin Boundaries in FeSe

Can-Li Song,[1,2,3] Yi-Lin Wang,[1] Ye-Ping Jiang,[1,2] Lili Wang,[1] Ke He,[1] Xi Chen,[2] Jennifer E. Hoffman,[3] Xu-Cun Ma,[1,*] and Qi-Kun Xue[1,2,†]




C2 structures in FeSe (0.4% diff. a vs b)

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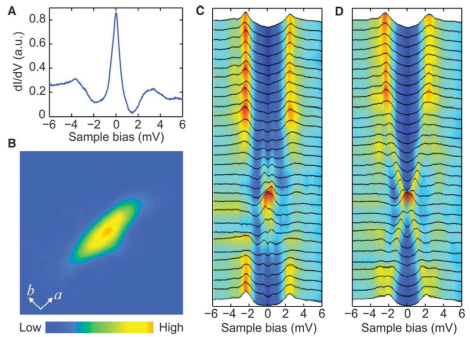


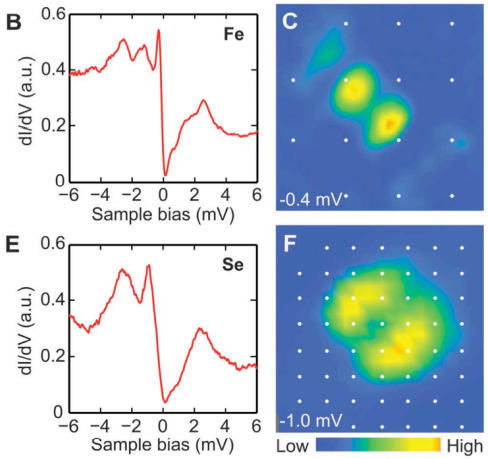


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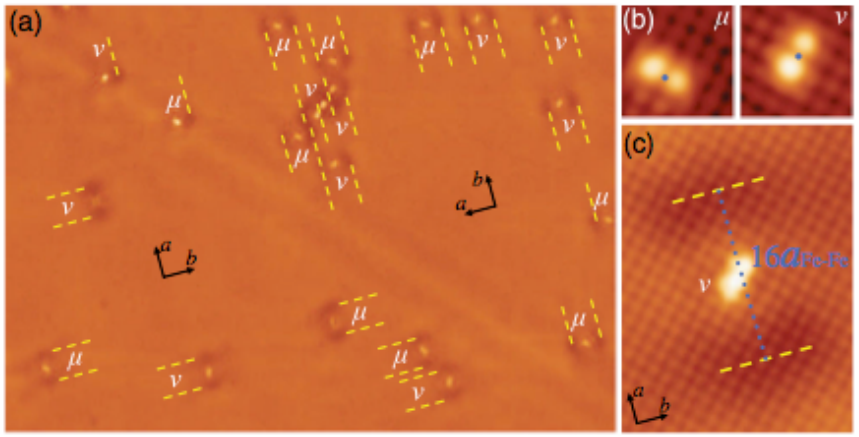
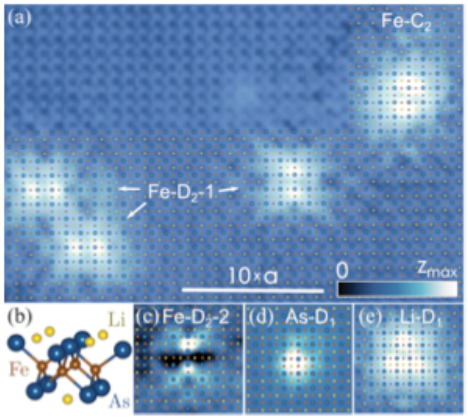


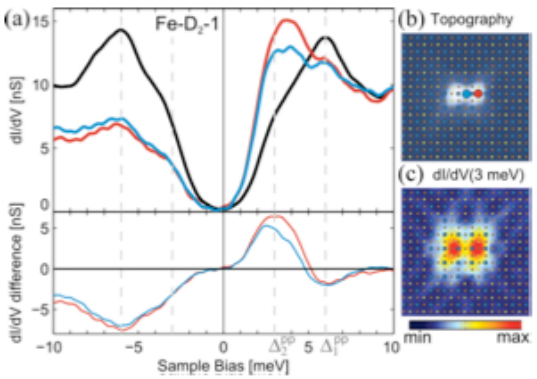

In SDW phase -> nematogens (see later in talk)

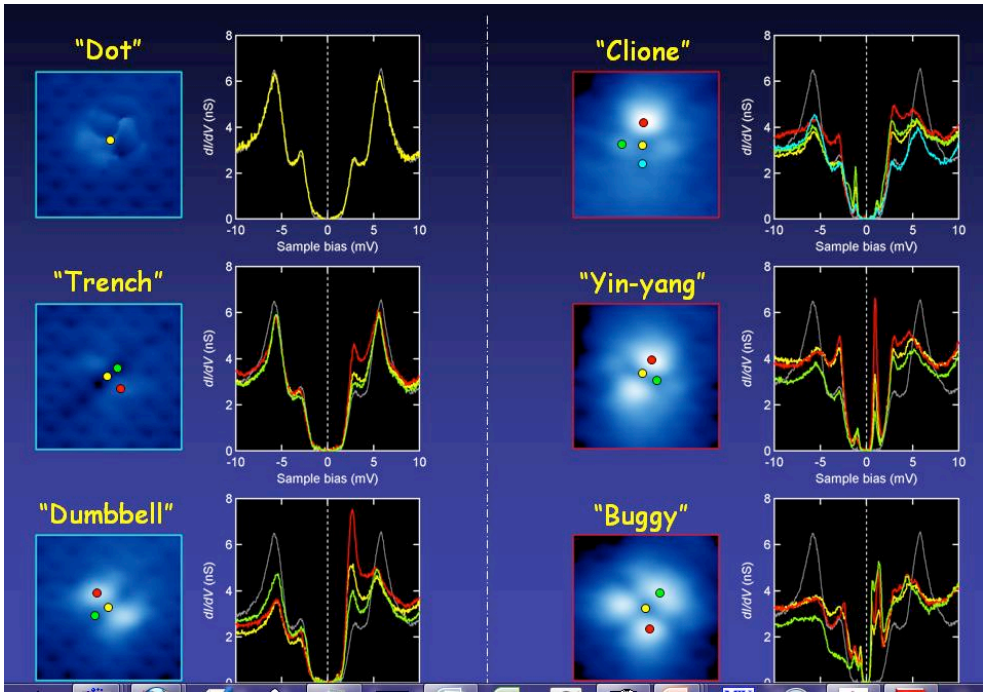
PHYSICAL REVIEW B **86**, 174503 (2012)

**Bound states of defects in superconducting LiFeAs studied by scanning tunneling spectroscopy**

S. Grothe,[1,2] Shun Chi,[1,2] P. Dosanjh,[1,2] Ruixing Liang,[1,2] W. N. Hardy,[1,2] S. A. Burke,[1,3,2] D. A. Bonn,[1,2] and Y. Pennec[1,2]




T. Hanaguri (preprint)

For many more details see e.g. J. Hoffman, Rep. Prog. Phys. 2011

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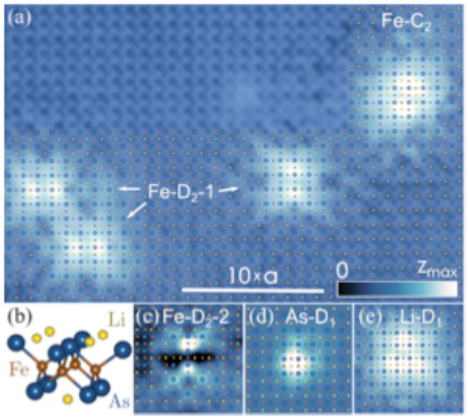


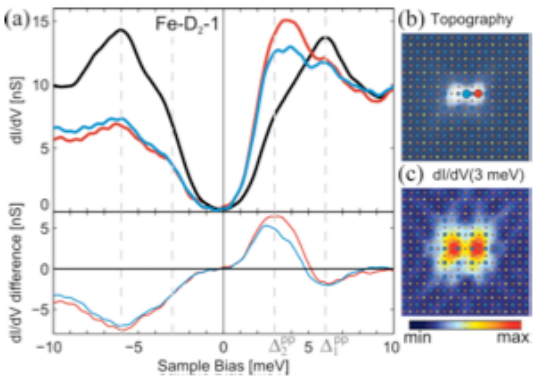


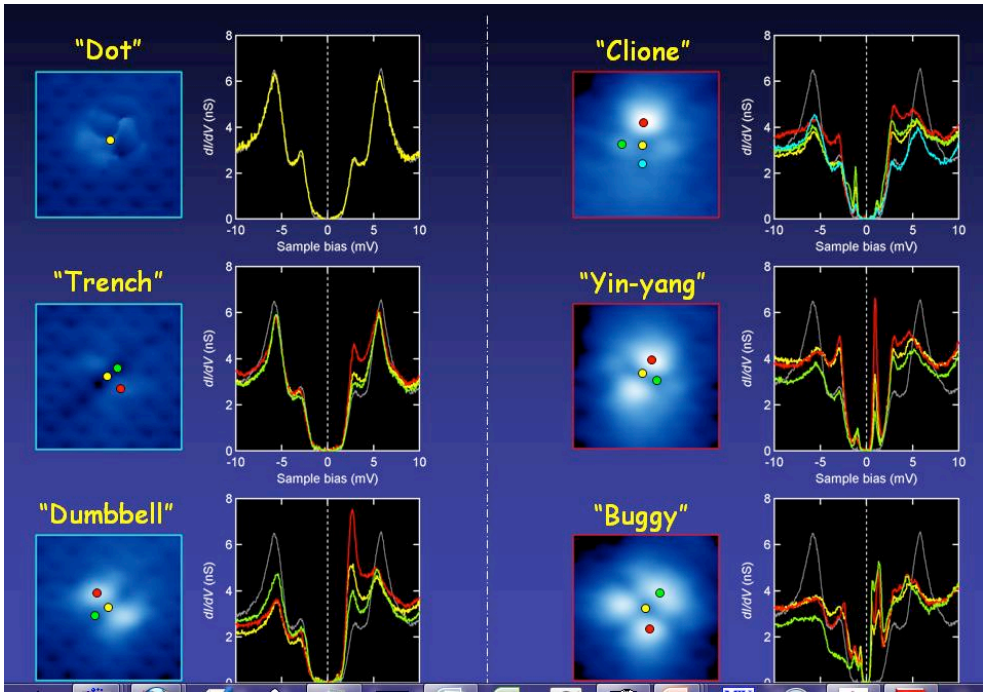


T. Hanaguri (preprint)

Single-impurity complexity

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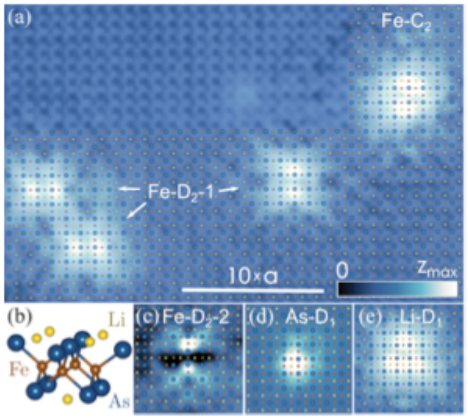


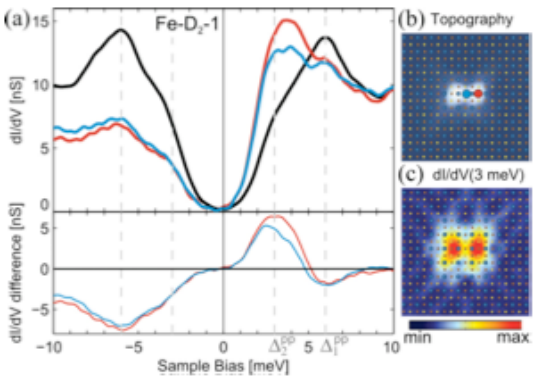


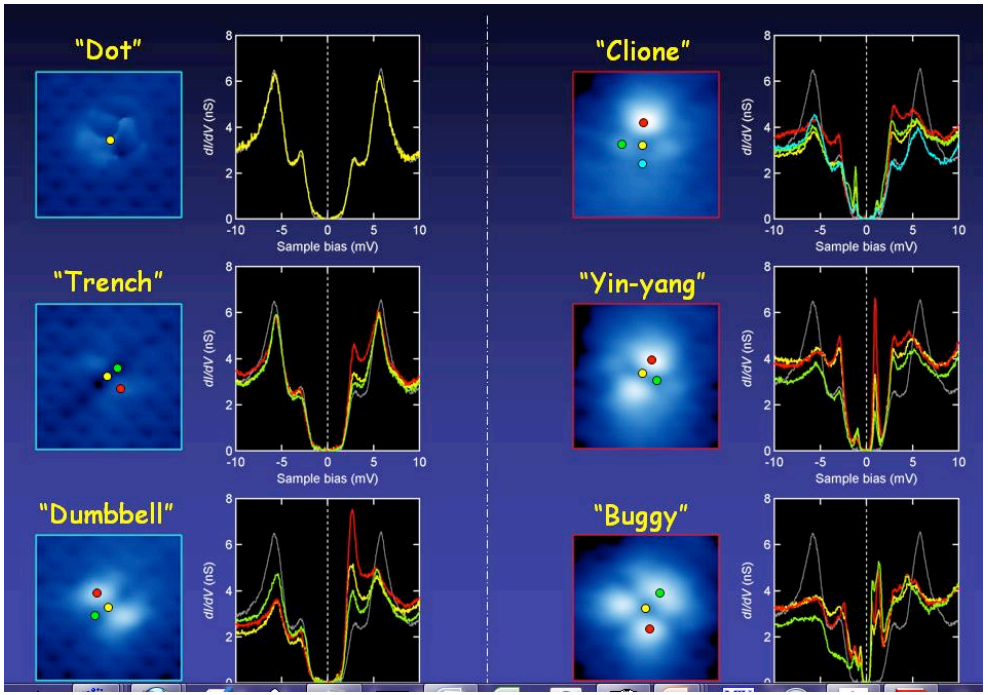


T. Hanaguri (preprint)

What do these data tell us of the underlying ground state?

# Theoretical status on bound states in s±

Bound states exist for s± but controversy about their position/weight

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**Impurity states in multiband $s$-wave superconductors: analysis of iron pnictides**

R. Beaird,[1] I. Vekhter,[1] and Jian-Xin Zhu[2]

[1] *Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA*

[2] *Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

(Dated: November 6, 2012)

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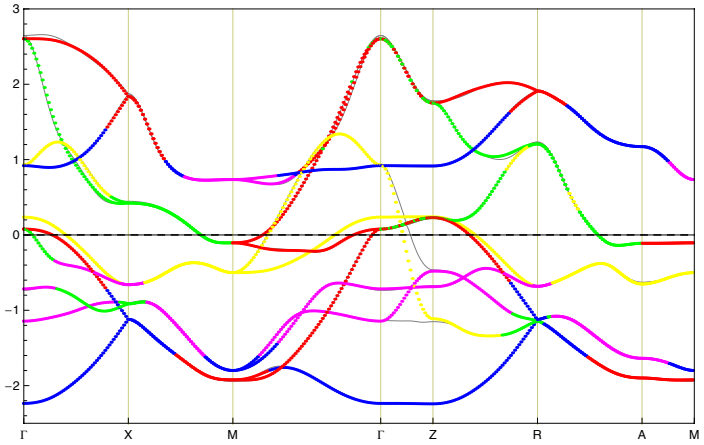
↓

Realistic modeling necessary

# Theoretical study of impurity states in the superconducting phase

$$H = H_0 + H_{int} + H_{BCS} + H_{imp},$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t^{\mu\nu}_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\mu\sigma} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}.$$




LiFeAs 111

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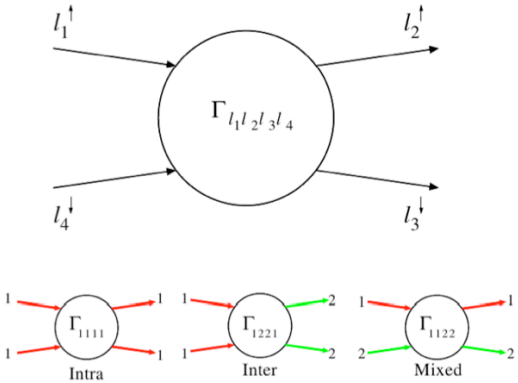


The pairing vertex in the singlet channel:

$$\Gamma_{pqst}(k-k',0) = \left[\frac{3}{2}U^s\chi_s^{RPA}(k-k',0)U^s + \frac{1}{2}U^s - \frac{1}{2}U^c\chi_c^{RPA}(k-k',0)U^c + \frac{1}{2}U^c\right]^{st}_{pq}$$

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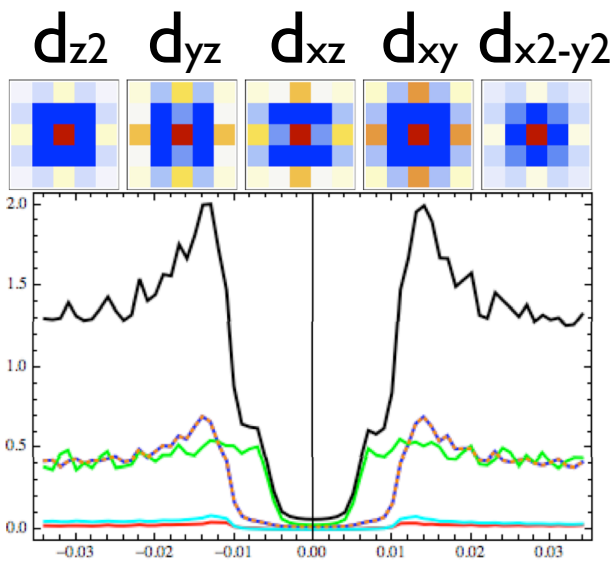
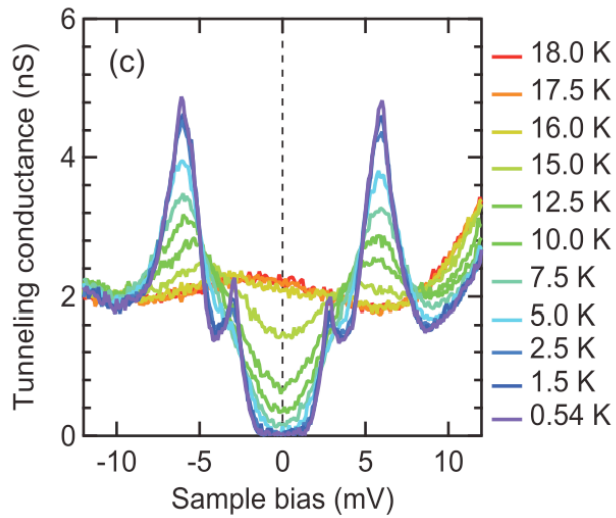
$$V^{\mu\nu}_{\mathbf{ij}} = \sum_{\mathbf{q}} \Gamma_{\mu\nu\mu\nu}(\mathbf{q}) \exp(i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j))$$




T. Hanaguri et al
PRB 2012

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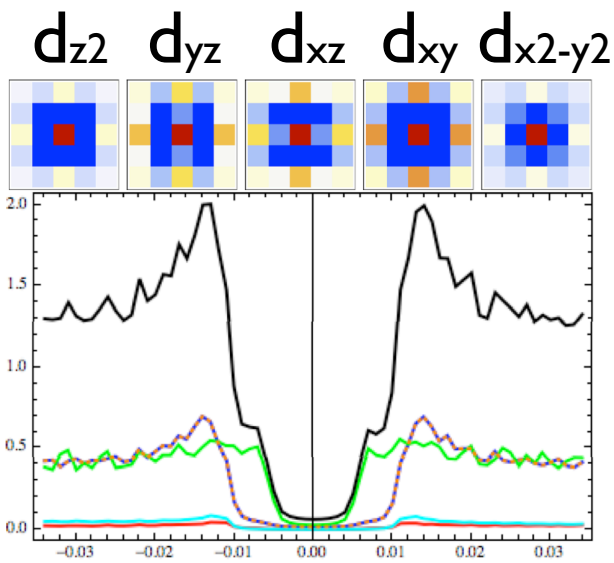


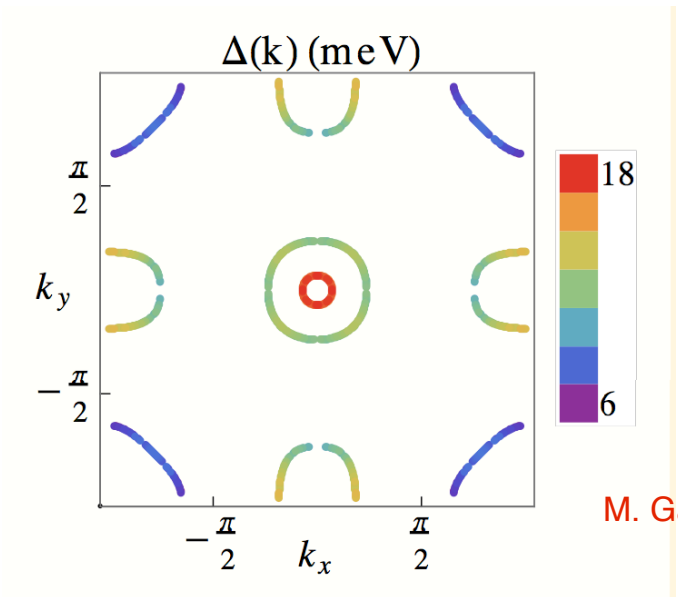


M. Gastiasoro *et al*, *preprint*

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Theoretical study of impurity states in the superconducting phase

$$H = H_0 + \cancel{H_{int}} + H_{BCS} + H_{imp},$$

First study (uncorrelated) superconducting state

# Theoretical study of impurity states in the superconducting phase

PHYSICAL REVIEW B **86**, 214512 (2012)

**Unexpected weak spatial variation in the local density of states induced by individual Co impurity atoms in superconducting $Na(Fe_{1-x}Co_x)As$ crystals revealed by scanning tunneling spectroscopy**

Huan Yang,[1] Zhenyu Wang,[2] Delong Fang,[1] Sheng Li,[1] Toshikaze Kariyado,[3] Genfu Chen,[2]
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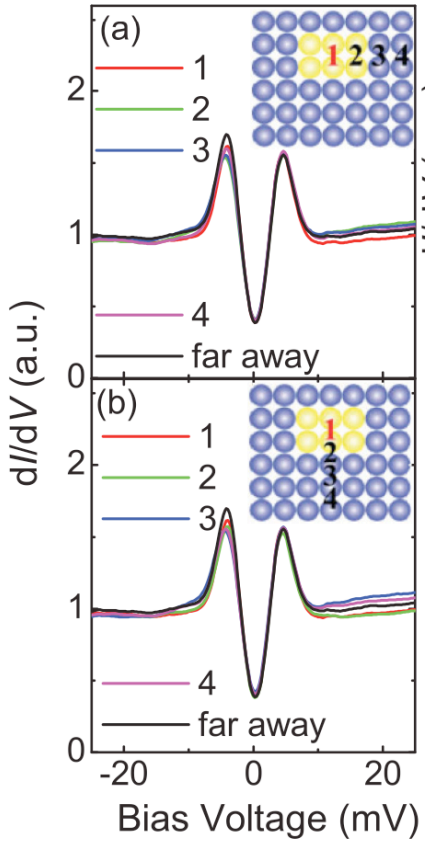


$$H_{imp} = \sum_{\mathbf{i}^* \mu\sigma} V_{imp}^{\mu\sigma} c^{\dagger}_{\mathbf{i}^* \mu\sigma} c_{\mathbf{i}^* \mu\sigma},$$

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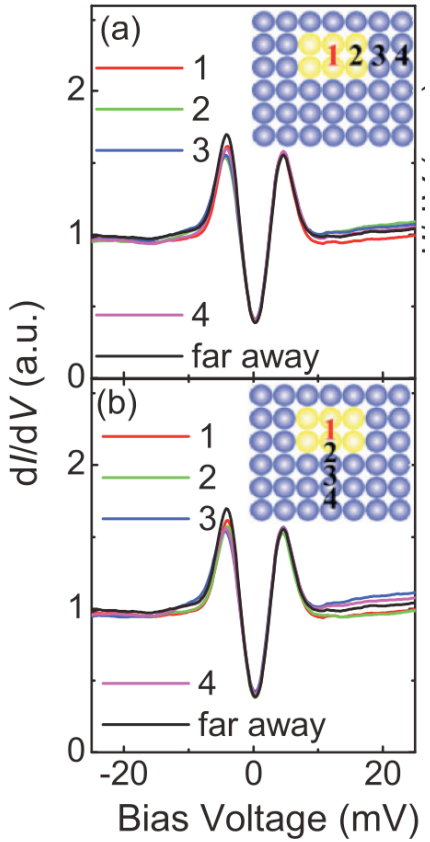
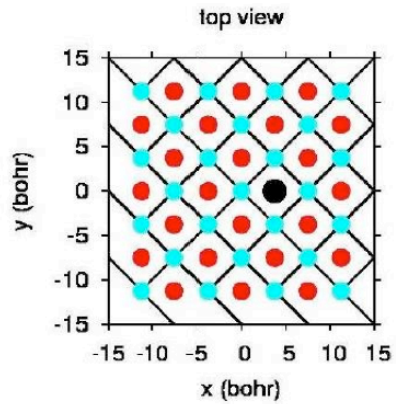



First-principles in $Ba(Fe_{1-x}Co_x)_2As_2$




| | | | | |
|---|---|---|---|---|
| −507 | 0 | 0 | 0 | 0 |
| 0 | −448 | 0 | 0 | 0 |
| 0 | 0 | −448 | 0 | 0 |
| 0 | 0 | 0 | −415 | 0 |
| 0 | 0 | 0 | 0 | −488 |

T. Berlijn, private communication

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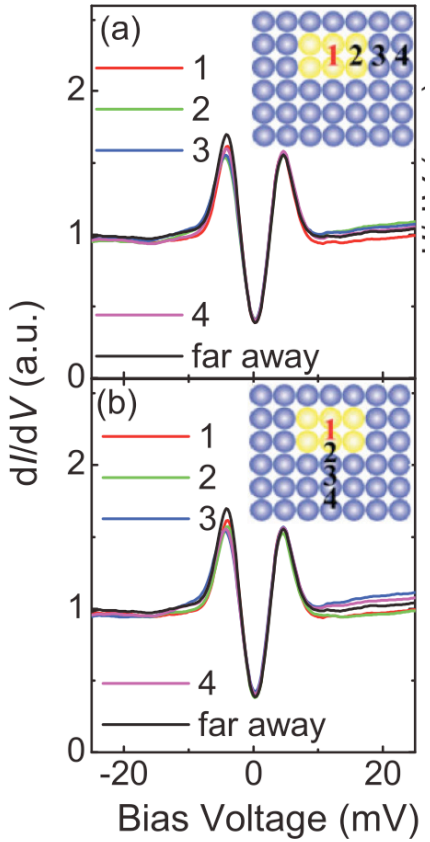


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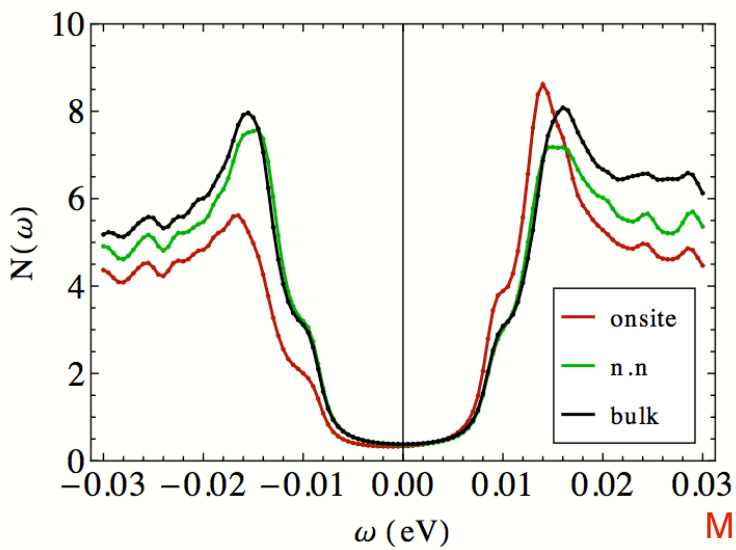
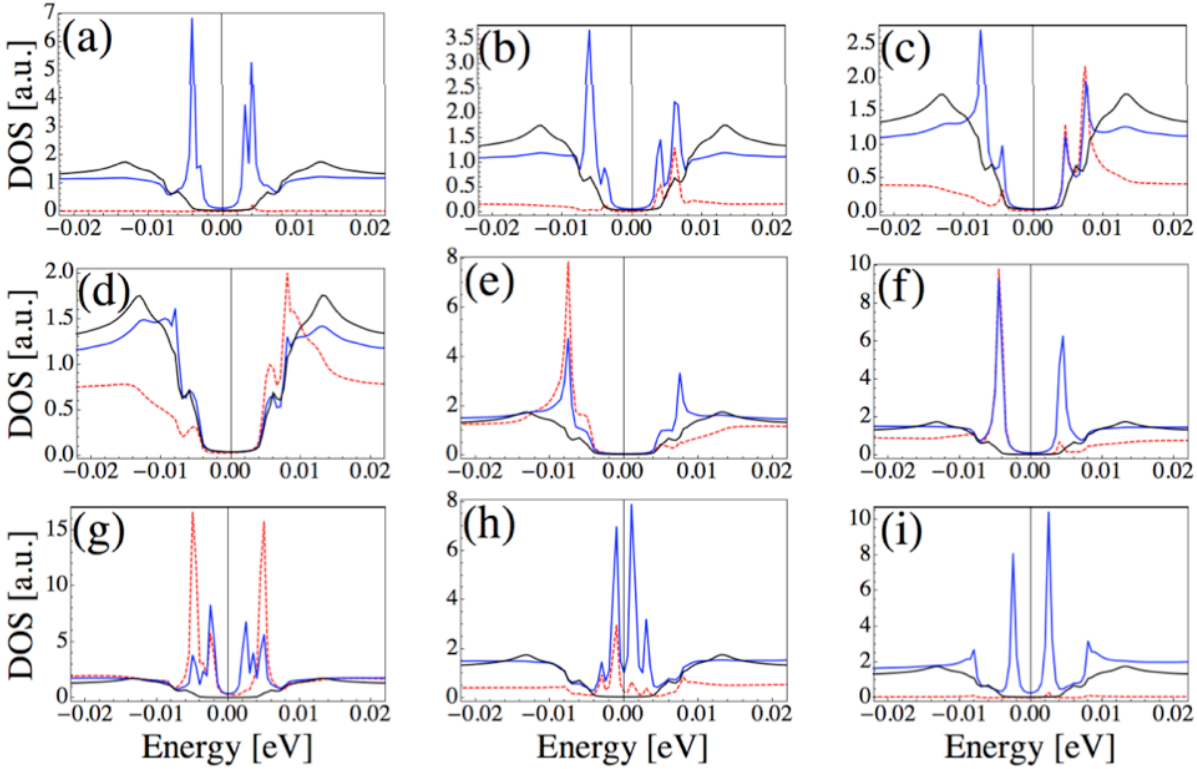


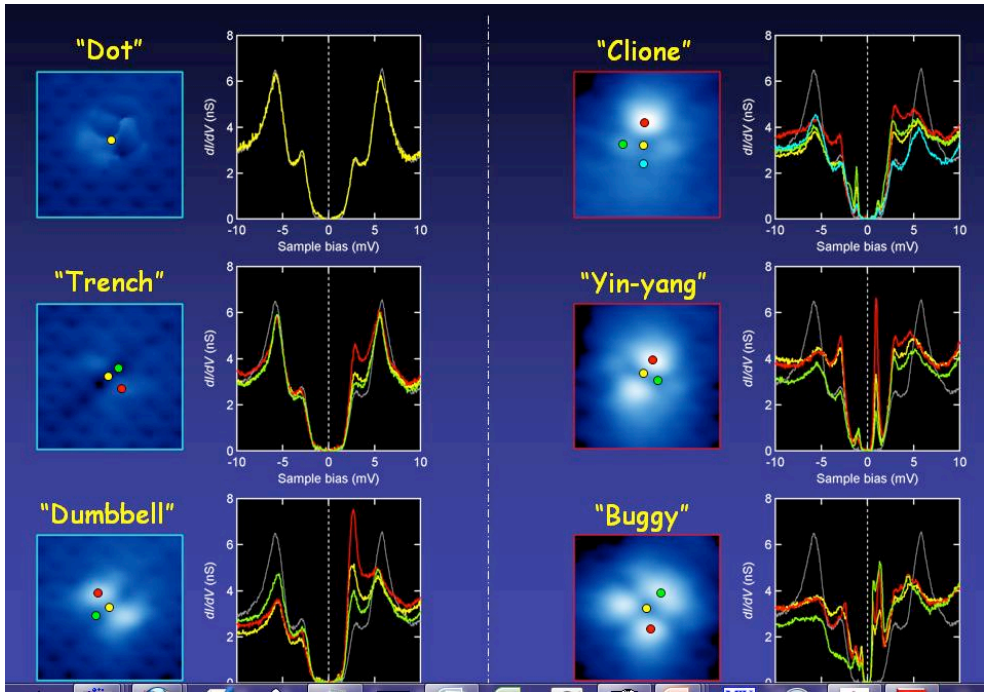

M. Gastiasoro *et al*, preprint 2013

# Five band model: nonmagnetic impurity $V_{imp}$ dependence




Consistent with Kariyado & Ogata, JPSJ 2010

FIG. 2. (Color online) Total LDOS for nonmagnetic point-like scatterers at the impurity site (dashed red line) and at the NN site (solid blue line). Panels (a-i) correspond to $V_{imp}/t = -8.0, -2.0, -1.0, -0.5, 0.5, 1.0, 1.5, 2.0, 8.0$. In all plots the solid black line is the DOS of the clean superconductor.




T. Hanaguri (preprint)

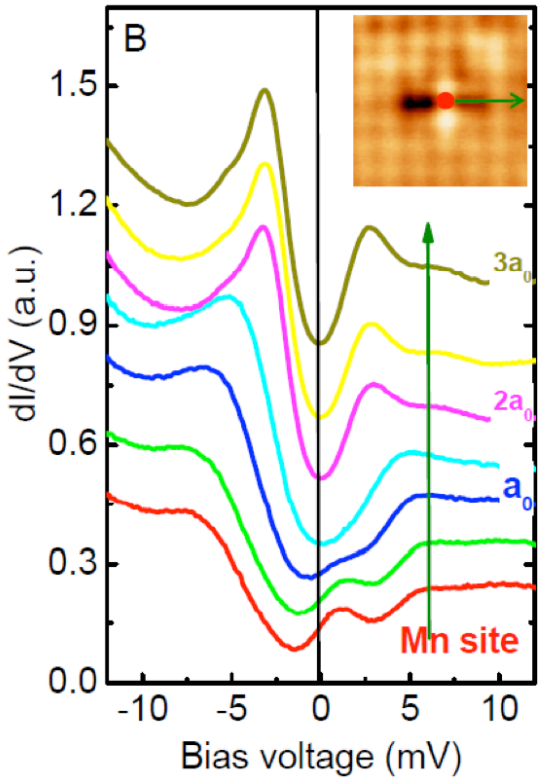
# Recent STM data from magnetic Mn impurities

**In-Gap Quasiparticle Excitations Induced by Non-Magnetic Cu Impurities in**

**$Na(Fe_{0.96}Co_{0.03}Cu_{0.01})As$ Revealed by Scanning Tunneling Spectroscopy**

Huan Yang[1†], Zhenyu Wang[2†], Delong Fang[1†], Qiang Deng[1], Qiang-Hua Wang[1],

Yuan-Yuan Xiang[1], Yang Yang[1], Hai-Hu Wen[1*]



# Five band model: magnetic impurity

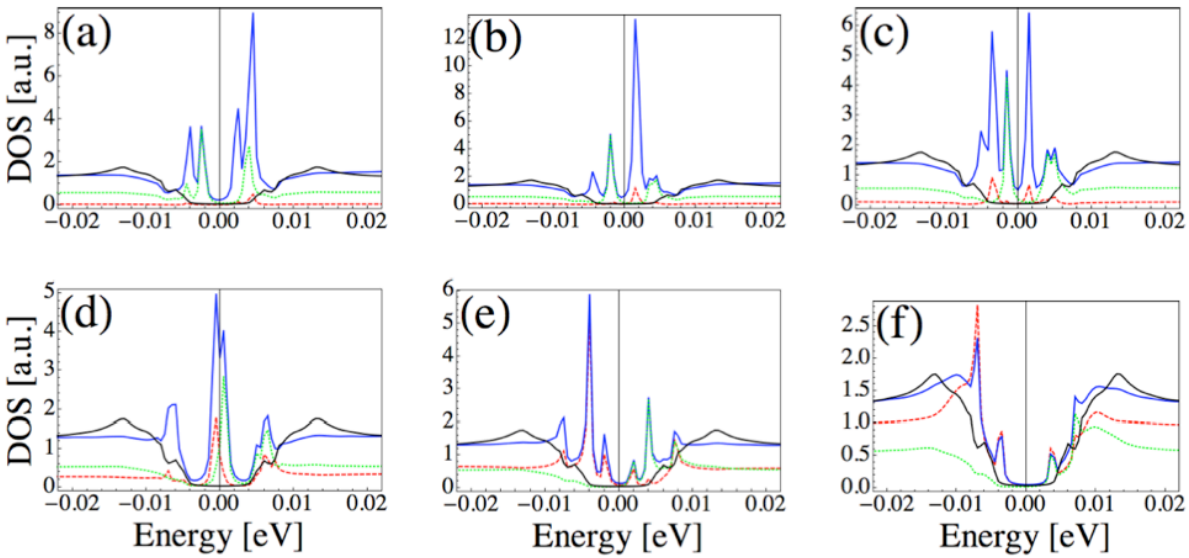
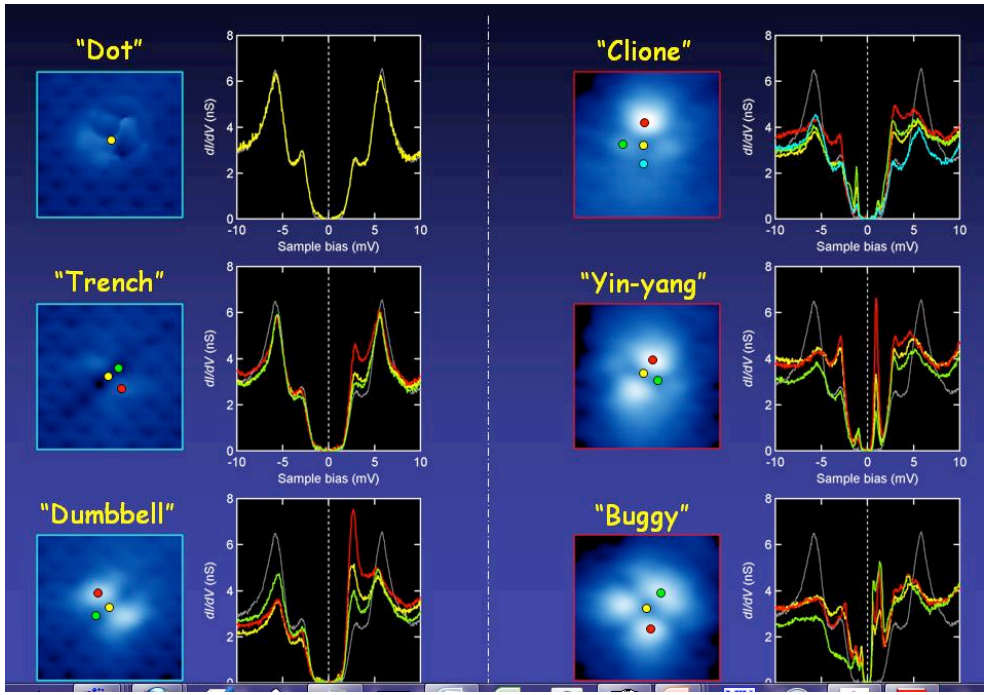



FIG. 3. (Color online) Total LDOS for magnetic point-like scatterers at the impurity site (dashed red lines) and at the NN site (solid blue line). The dotted green lines show the spin-up LDOS at the NN site. Panels (a-f) correspond to $V_{imp}/t = -8.0, -6.0, -4.0, -2.0, -1.0, -0.5$. Repulsive potentials lead to the same total LDOS (with interchanged spin-polarisation of the individual bound states).




T. Hanaguri (preprint)

If spin-resolved STM finds that one of these 3 are nonmagnetic -> strong evidence for s±

# Five band model

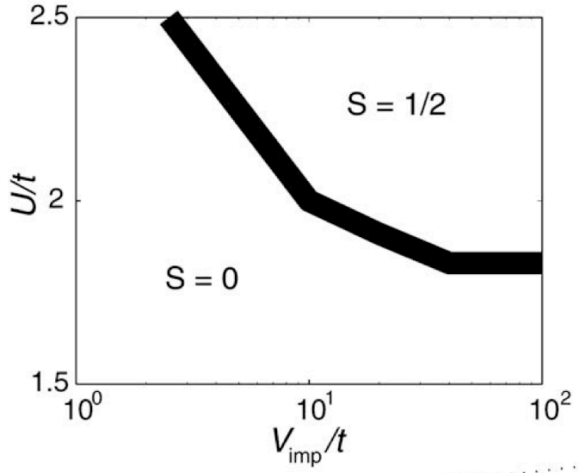
$$H = H_0 + H_{int} + H_{BCS} + H_{imp},$$

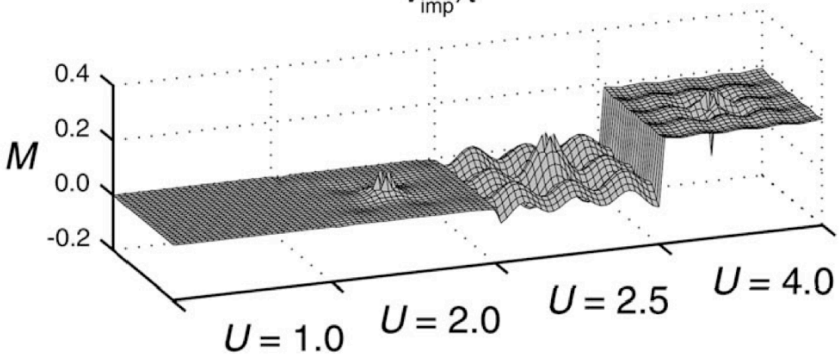
What happens when we include correlations?

$$H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'}$$

$$- 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c^{\dagger}_{\mathbf{i}\mu\sigma} c^{\dagger}_{\mathbf{i}\mu\bar{\sigma}} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma},$$

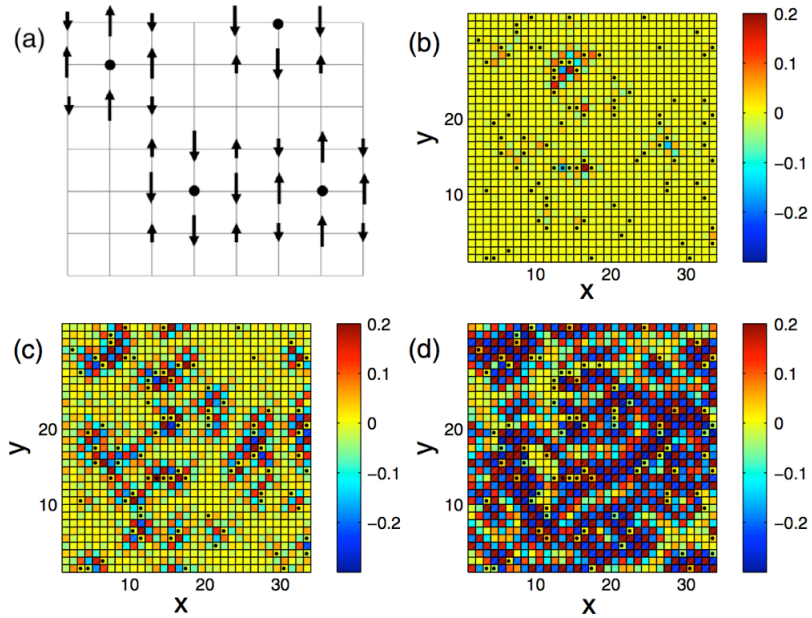
# Single (cuprate) band; impurity-induced order




J. Harter et al, PRB 2007

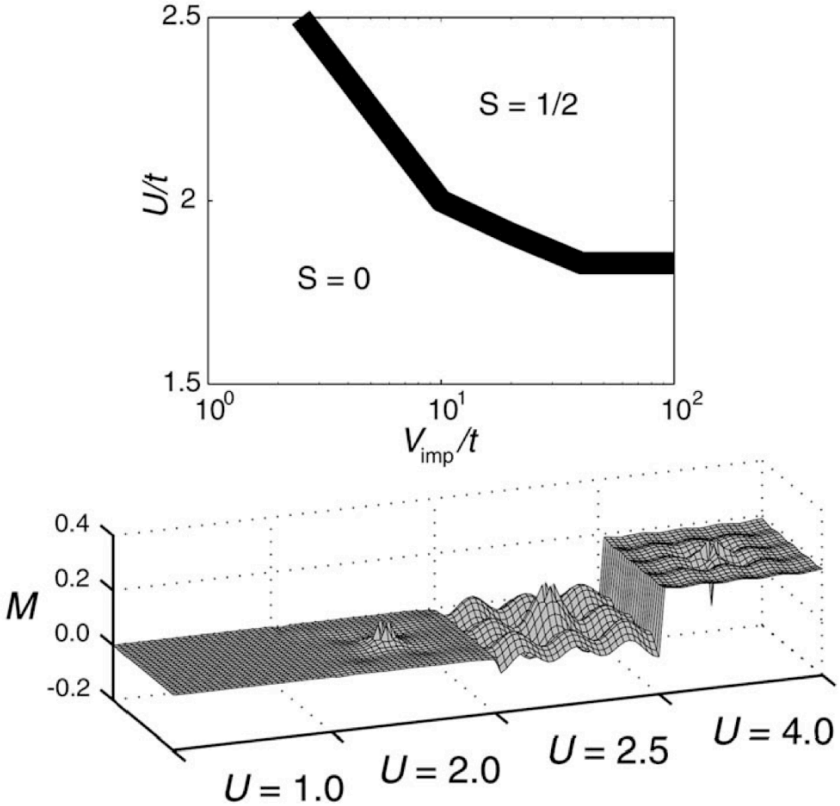
BMA et al, PRL 2007



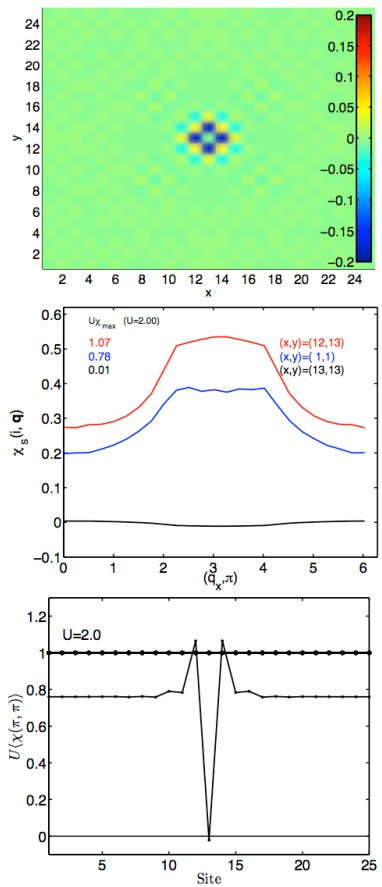

Proposed as spin-glass phase of e.g. LSCO

# Single (cuprate) band; impurity-induced order

Origin of disorder-induced magnetism:
local Stoner instability

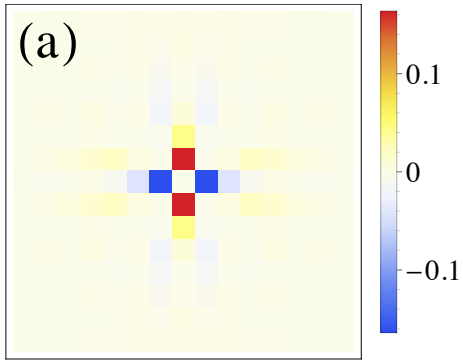



J. Harter et al, PRB 2007

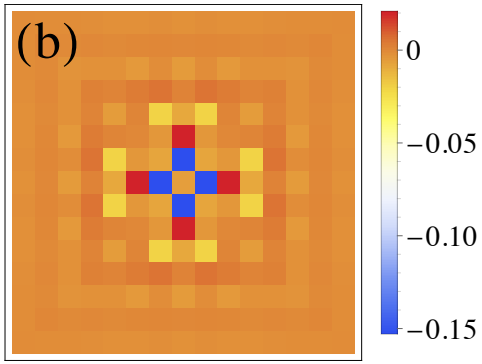



A. T. Rømer et al,
*preprint*

# Five band model: impurity-induced order in FeSC



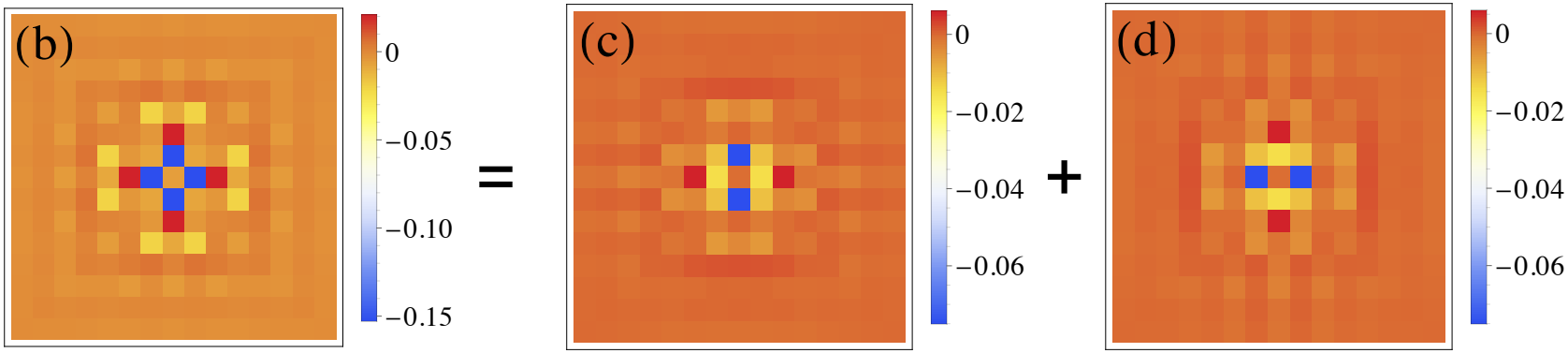

Disorder-induced orbital order



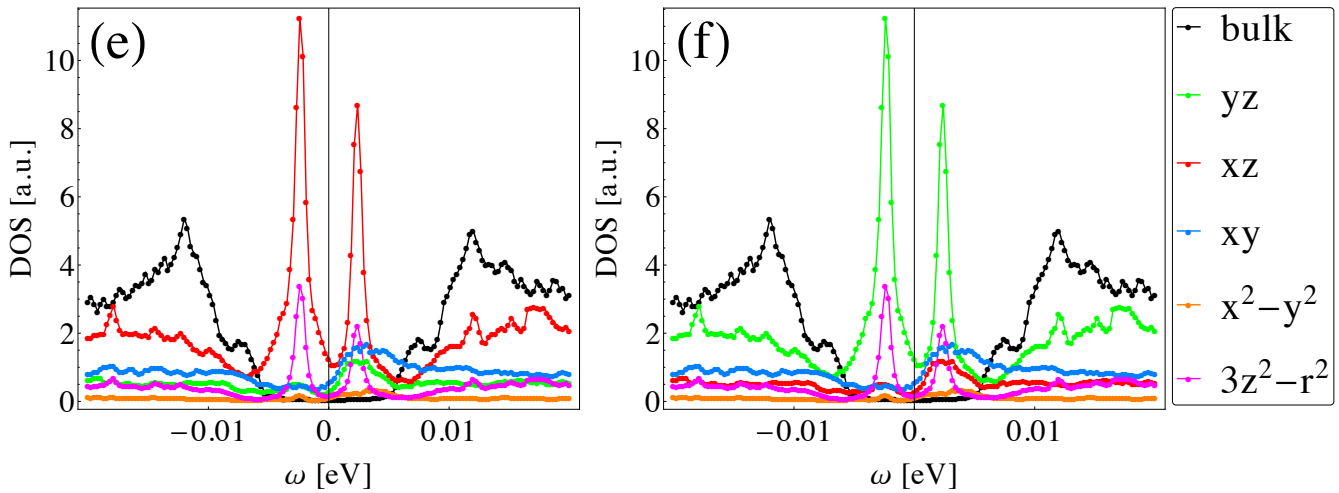

Disorder-induced magnetic order

M. Gastiasoro *et al*, *preprint*

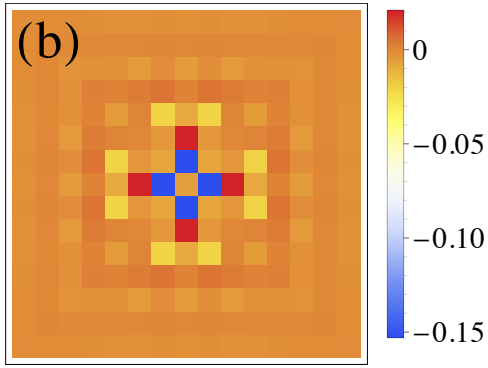
# Five band model: impurity-induced order in FeSC




Disorder-induced magnetic order due to local Stoner in xz & yz.



# Implications of induced order: spin glass phase




Disorder-induced magnetic order

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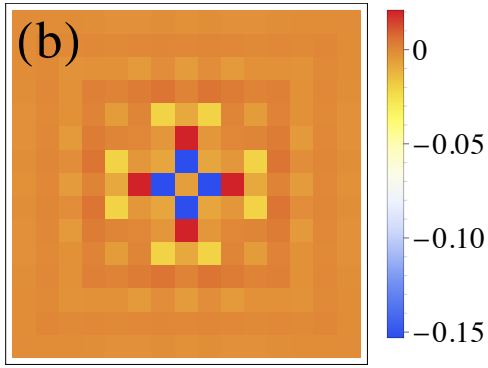
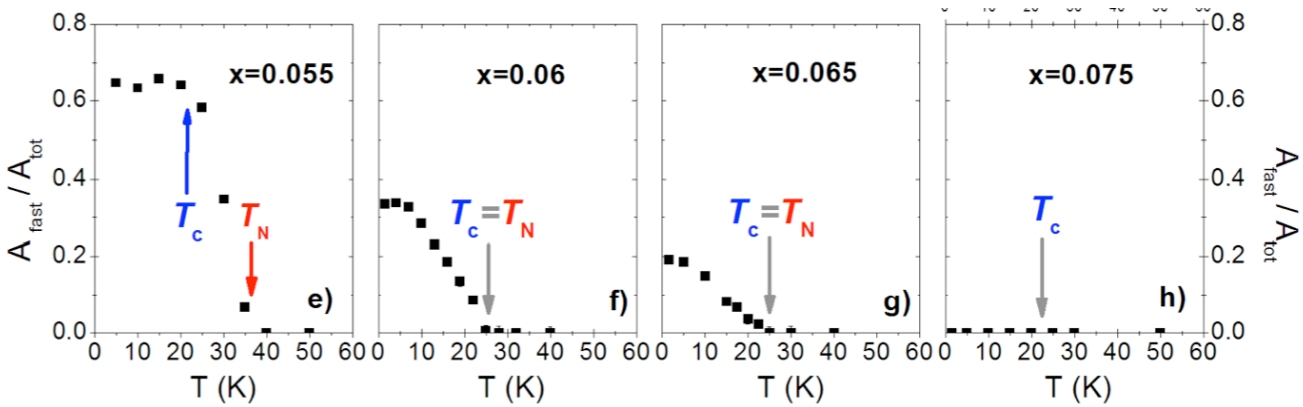



Disorder-induced magnetic order

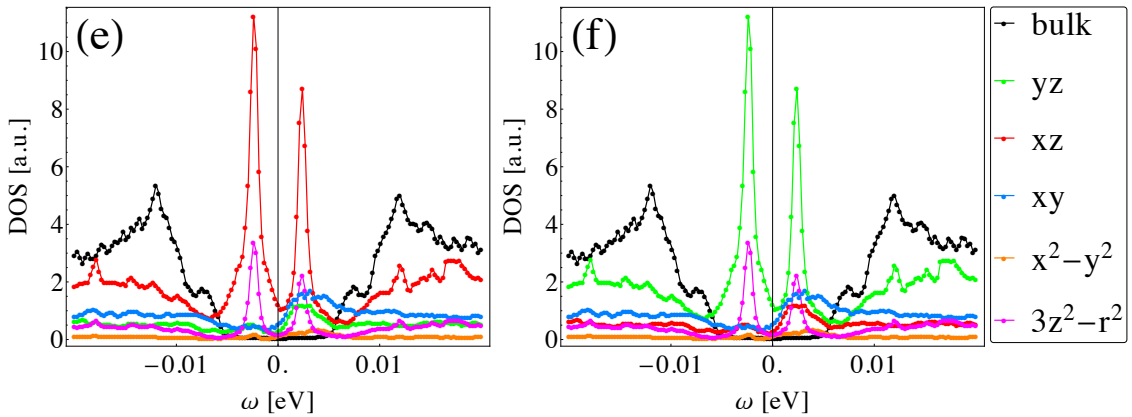
**Muon spin rotation study of magnetism and superconductivity in**

**$Ba(Fe_{1-x}Co_x)_2As_2$ single crystals**

C. Bernhard[1], C. N. Wang[1], L. Nuccio[1,2], L. Schulz[1*], O. Zaharko[3], J. Larsen[4], C. Aristizabal[2]
M. Willis[2], A. J. Drew[2], G. D. Varma[5], T. Wolf[6], and Ch. Niedermayer[3]



# Implications of induced order: spin glass phase




Disorder-induced magnetic order at T<Tc

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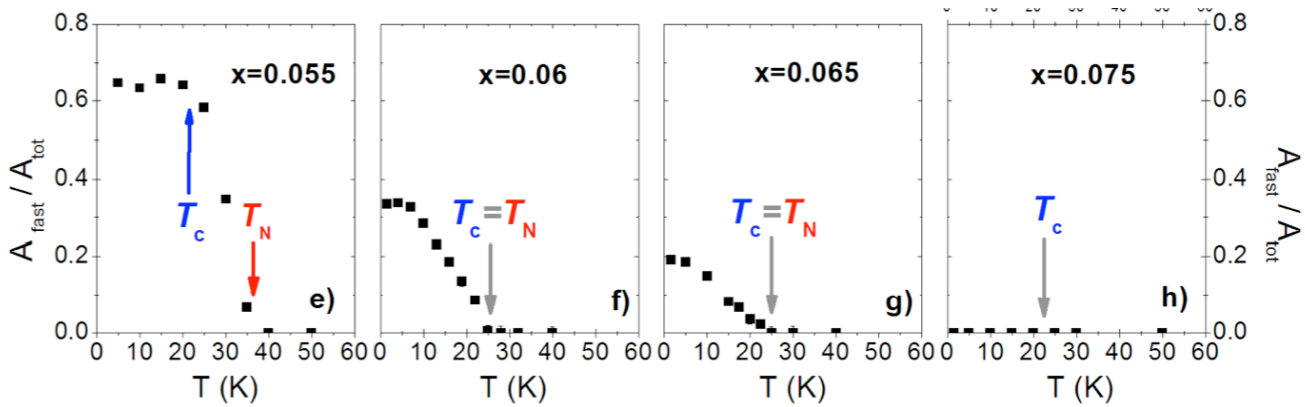

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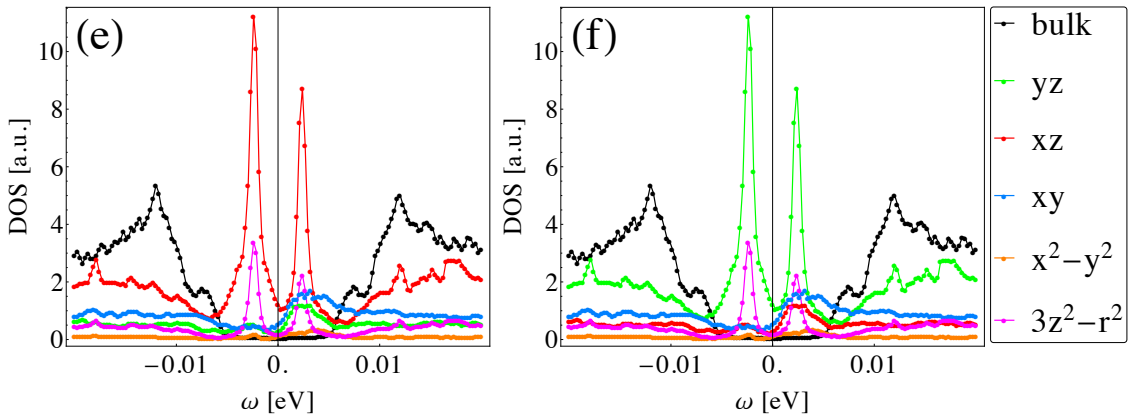


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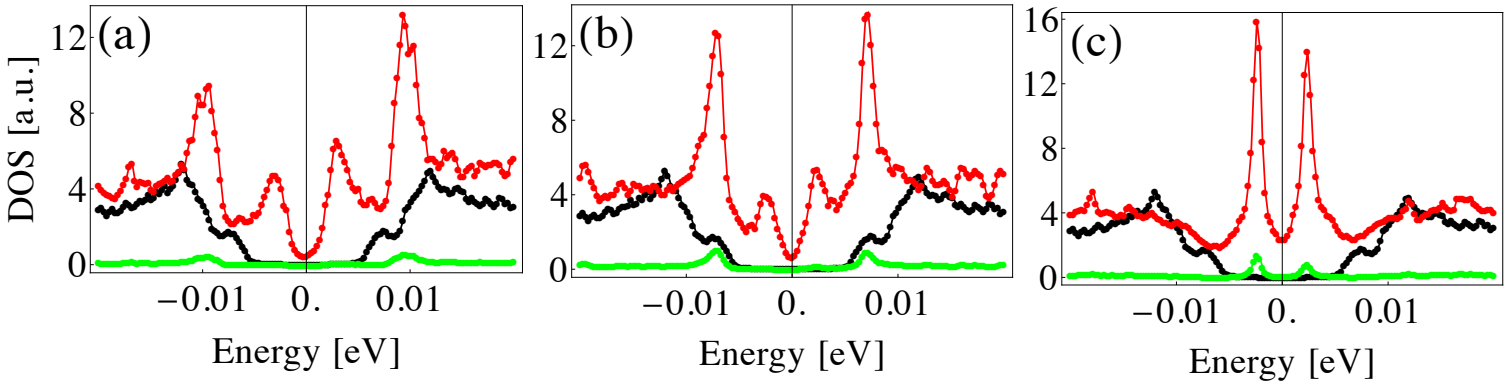
... Even in the strongly overdoped regime at $x = 0.11$, where the static magnetic order has disappeared, we find that the low energy spin fluctuations are anomalously enhanced below $T_c$. These findings point toward a drastic change in the relationship between the magnetic and superconducting orders from a competitive one in the strongly underdoped regime to a constructive one in near optimally and overdoped samples. ...

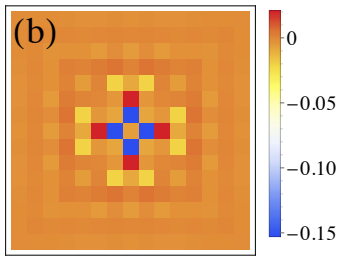
# Implications of induced order: LDOS



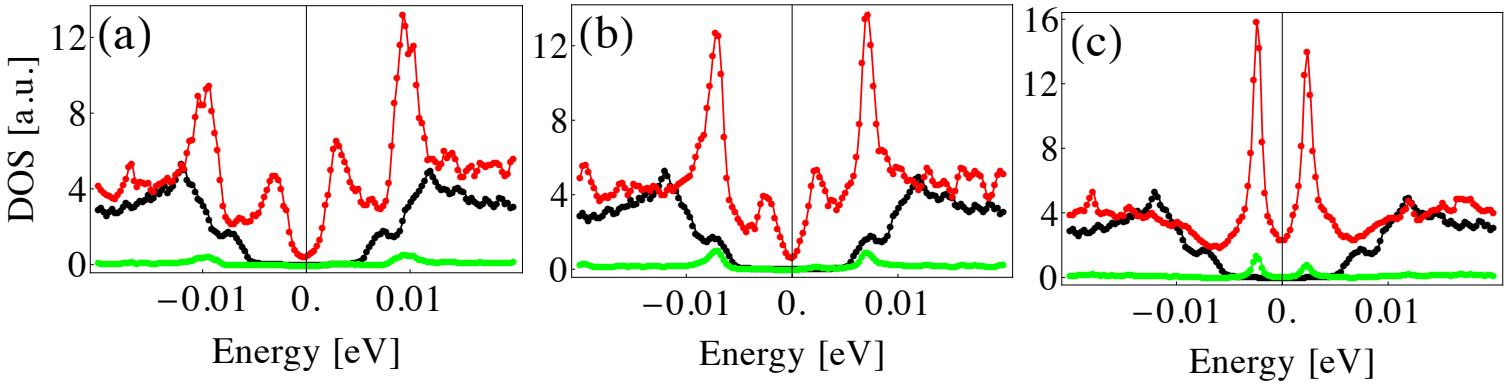

non-selfconsistent BdG

selfconsistent BdG

selfconsistent BdG with induced magnetic order



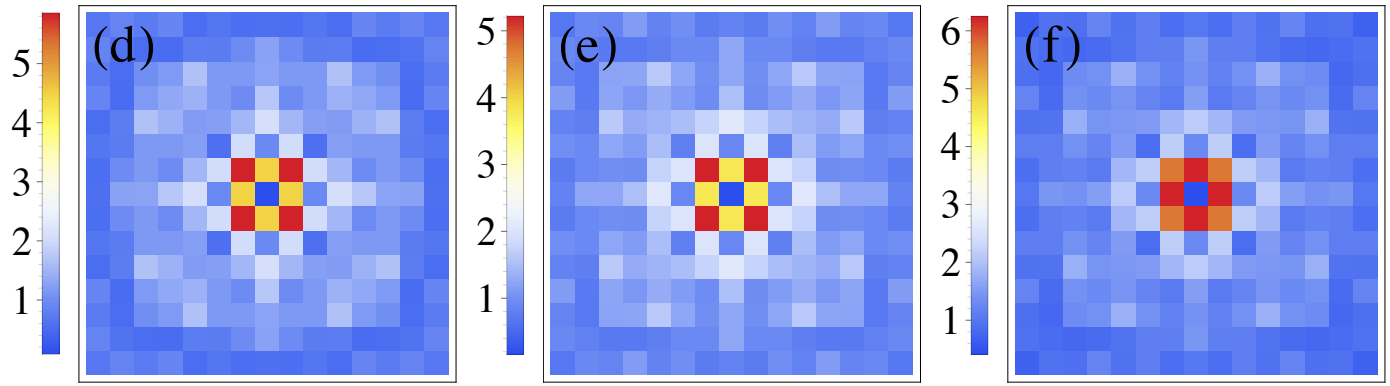
# Implications of induced order: LDOS




non-selfconsistent BdG

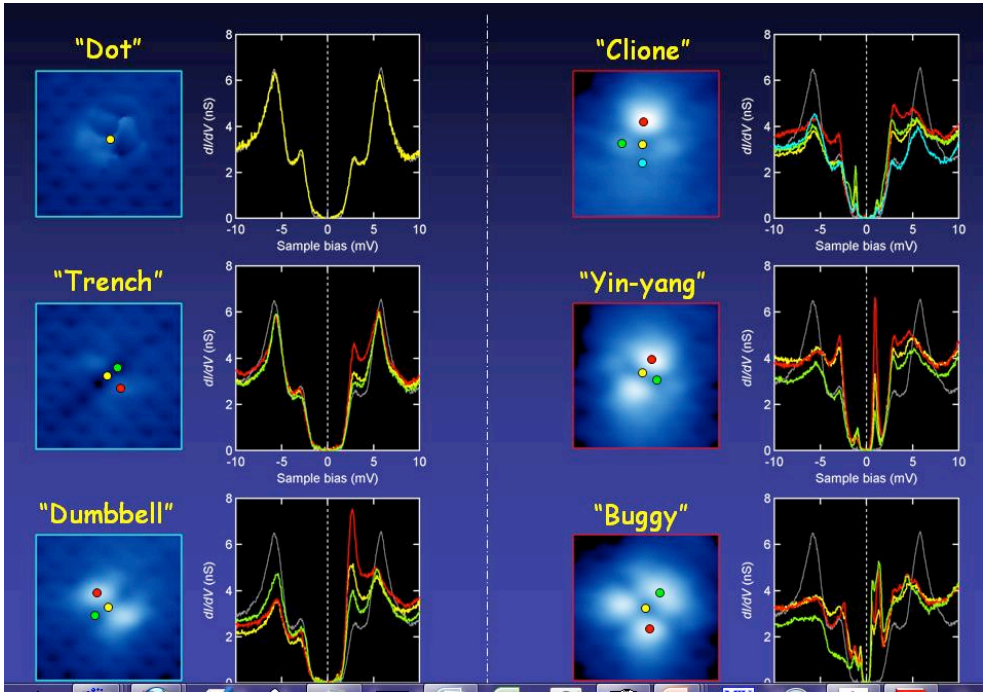
selfconsistent BdG

selfconsistent BdG with induced magnetic order




M. Gastiasoro *et al*, *preprint*

# Not there yet!




T. Hanaguri (preprint)

Need to include As, local structural modulations, associated Wannier w.f. etc

# Outline

1a) Overview of selected experimental data (STM)

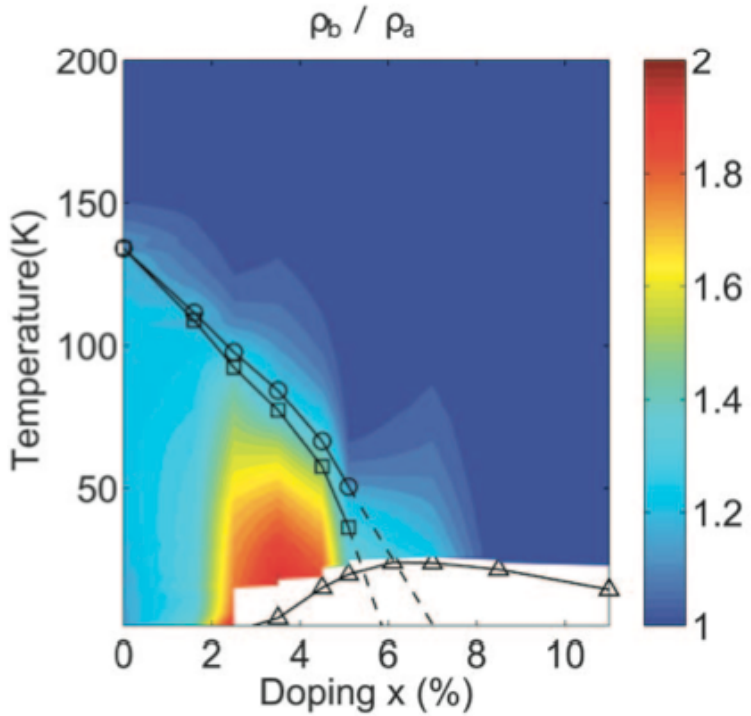
1b)Theoretical modeling:
- SC phase (realistic modeling of bound states)

2a) Overview of selected experimental data (STM, transport)

2b)Theoretical modeling:
- SDW phase (emergent impurity states, anisotropic scatterers)

3) Conclusions

# Resistivity anisotropy




Diminishing AF & Orthorhombicity

J. Chu et al
Science 2011

# What is the origin of the anisotropy/nematicity

1) Orbital ordering $n_{xz} \neq n_{yz}$

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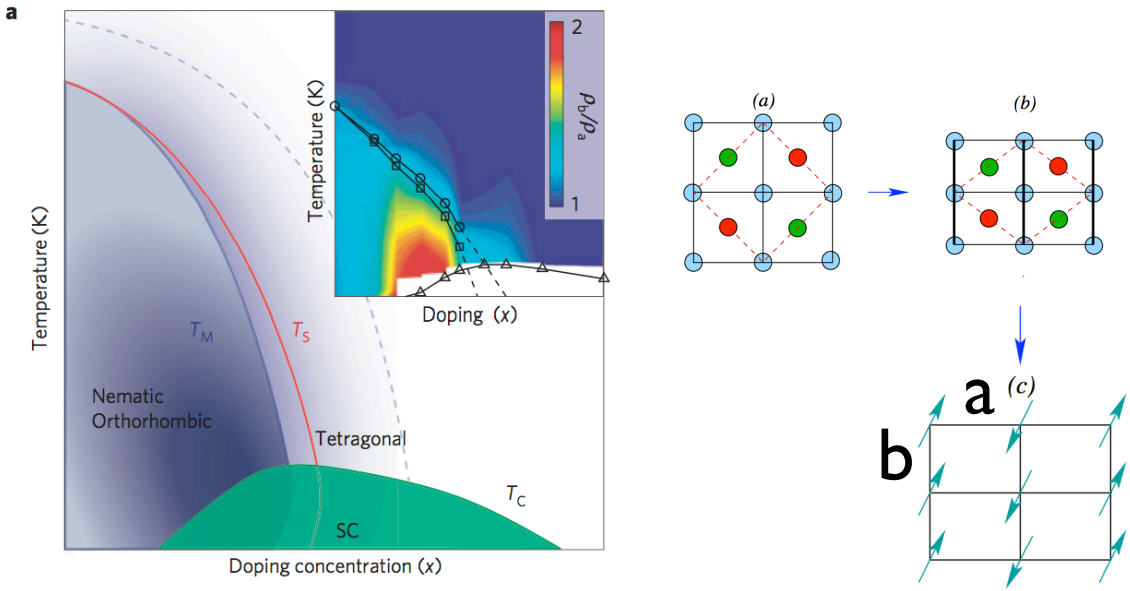
LETTERS
PUBLISHED ONLINE: 17 FEBRUARY 2013 | DOI: 10.1038/NPHYS2544
nature physics

# Anisotropic impurity states, quasiparticle scattering and nematic transport in underdoped $Ca(Fe_{1-x}Co_x)_2As_2$

M. P. Allan[1,2,3], T-M. Chuang[2,3,4,5], F. Massee[2,3,6], Yang Xie[2], Ni Ni[7,8], S. L. Bud'ko[7,8], G. S. Boebinger[5], Q. Wang[9], D. S. Dessau[9], P. C. Canfield[7,8], M. S. Golden[6] and J. C. Davis[2,3,10,11]*




Commensurate antiferromagnetism with orthorhombic crystal symmetry exists in the phase 'parent' to the superconductivity in most underdoped FeAs materials. The *a* axis unit cell is fractionally longer than that of the *b* axis, with the Fe spins aligning in an anti-parallel fashion along the *a* axis but parallel along the *b* axis.

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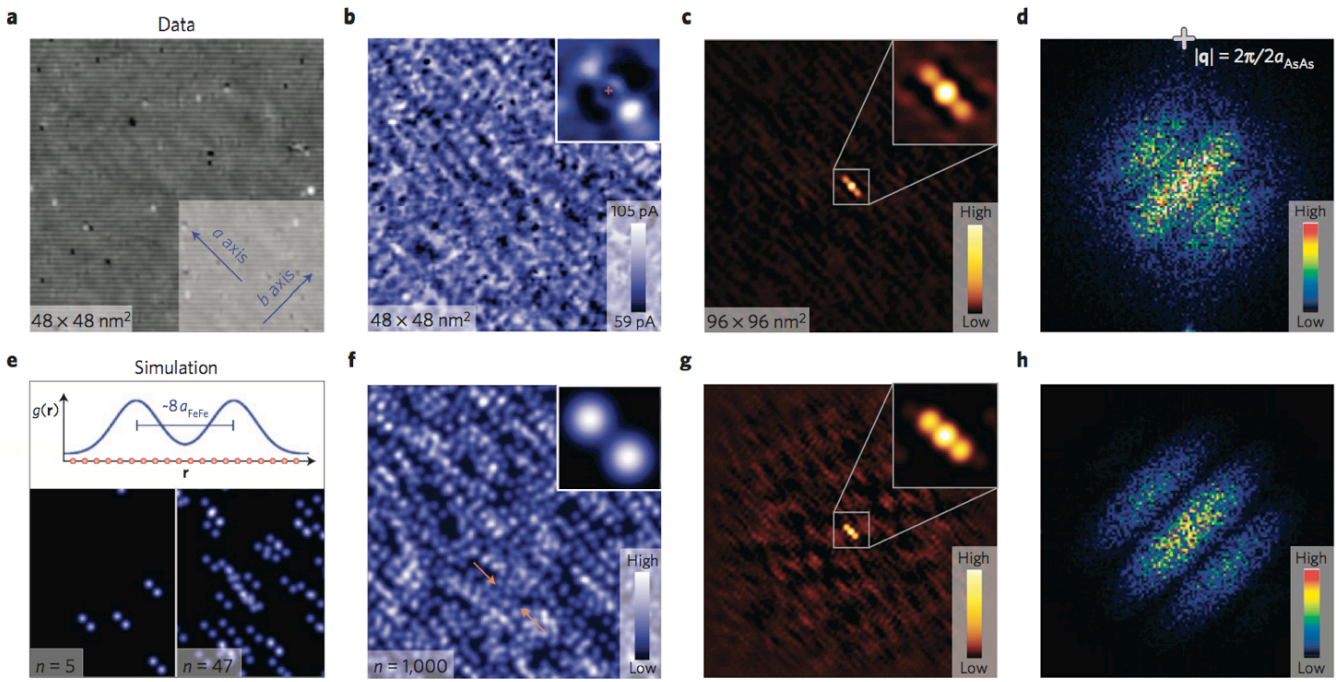


$$I(\mathbf{r}, -37\,\mathrm{meV}) = \int_0^{E\approx -37\,\mathrm{meV}} g(\mathbf{r}, \omega)\, \mathrm{d}\omega$$

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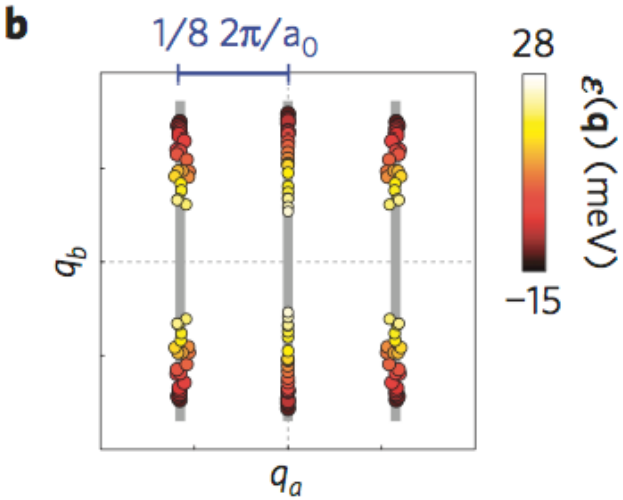


1D hole-like dispersion;
scattering off the dimers

1) Doping induced

2) Not SDW Fermi surface effect

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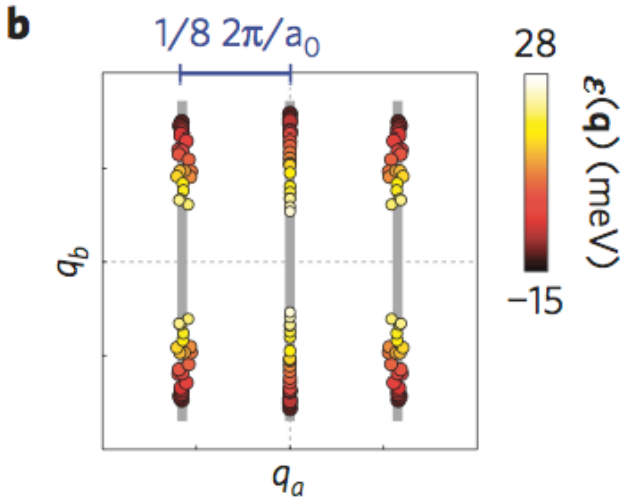


1D hole-like dispersion; scattering off the dimers

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$$P(\mathbf{q},E) = \frac{1}{N}\left|\frac{1}{\pi}\mathrm{Im}\Lambda(\mathbf{q},E)\right|^2 |\delta\varepsilon(\mathbf{q})|^2$$

Importance of structure factor

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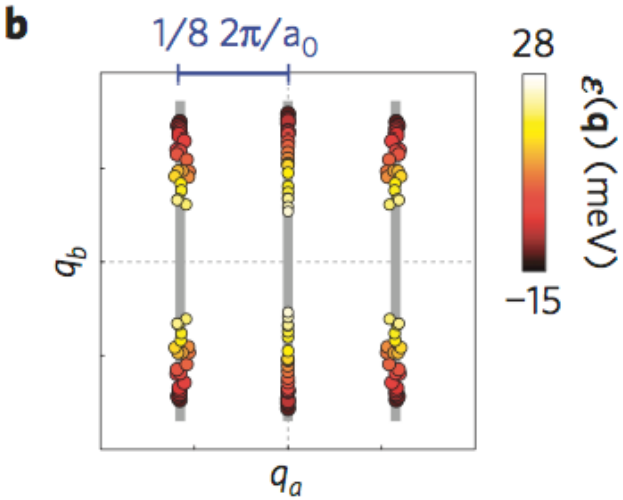


1D hole-like dispersion; scattering off the dimers

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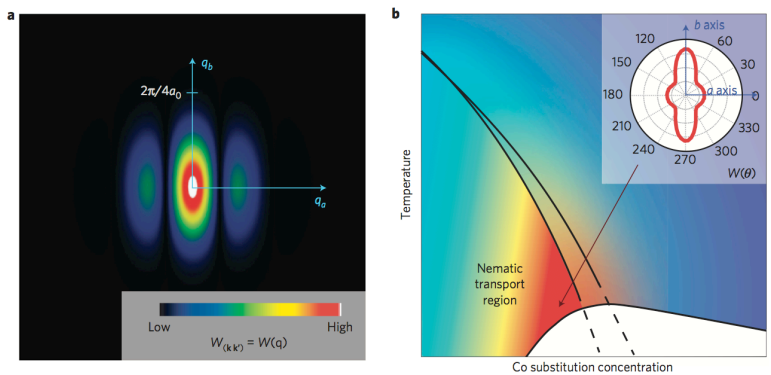


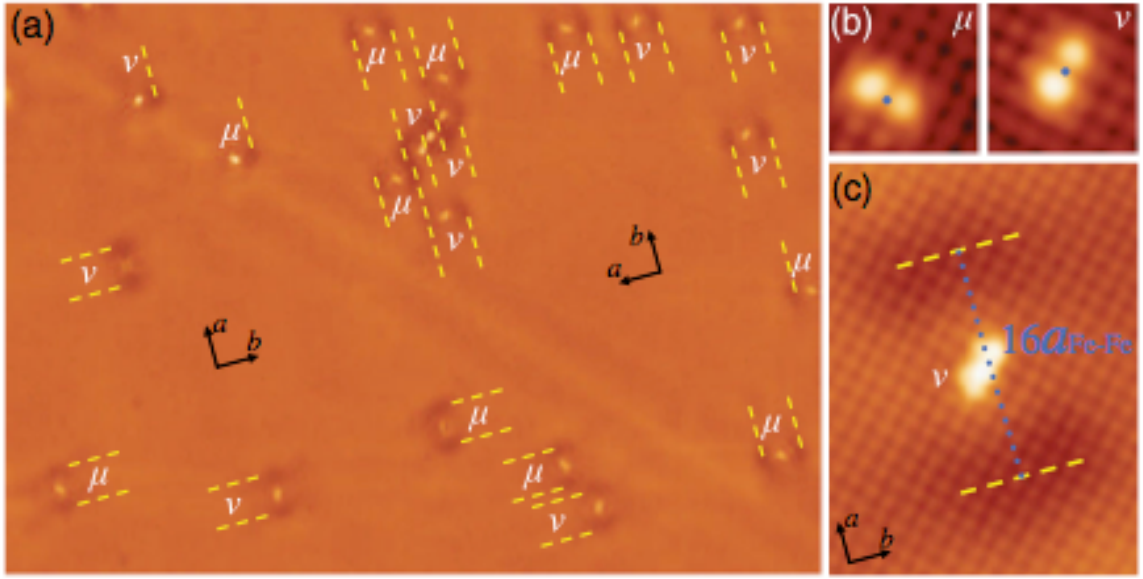

$\rho_b > \rho_a$

x dep.

PRL **109,** 137004 (2012) PHYSICAL REVIEW LETTERS week ending 28 SEPTEMBER 2012

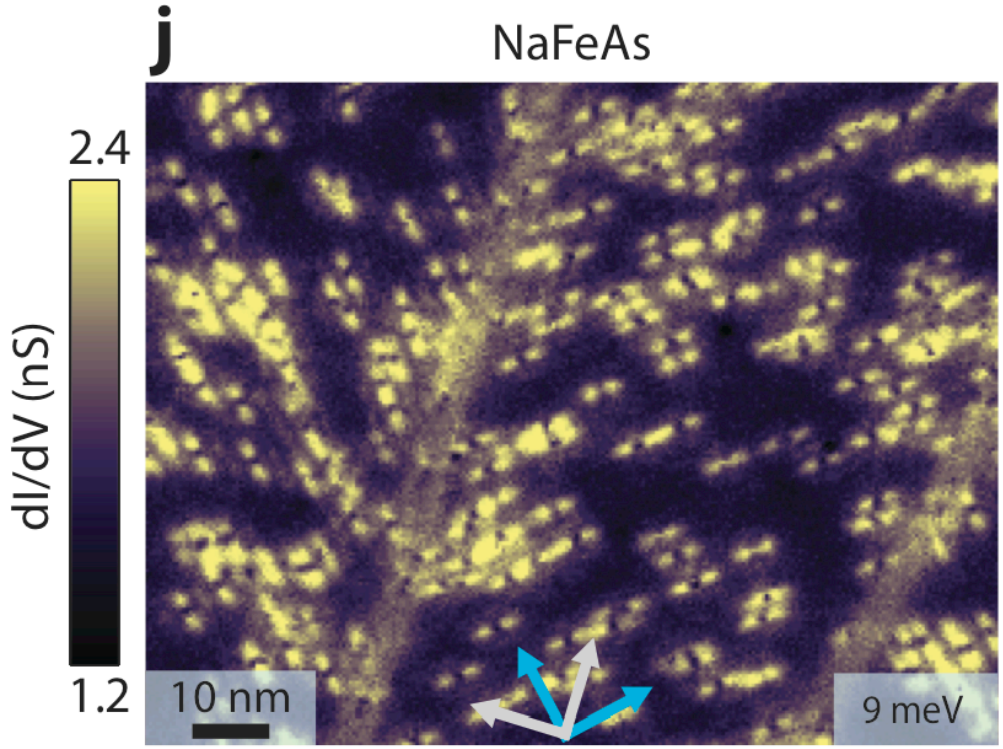
# Suppression of Superconductivity by Twin Boundaries in FeSe

Can-Li Song,[1,2,3] Yi-Lin Wang,[1] Ye-Ping Jiang,[1,2] Lili Wang,[1] Ke He,[1] Xi Chen,[2] Jennifer E. Hoffman,[3] Xu-Cun Ma,[1,*] and Qi-Kun Xue[1,2,†]



**Visualization of Electron Nematicity and Unidirectional Antiferroic Fluctuations at High Temperatures in NaFeAs**

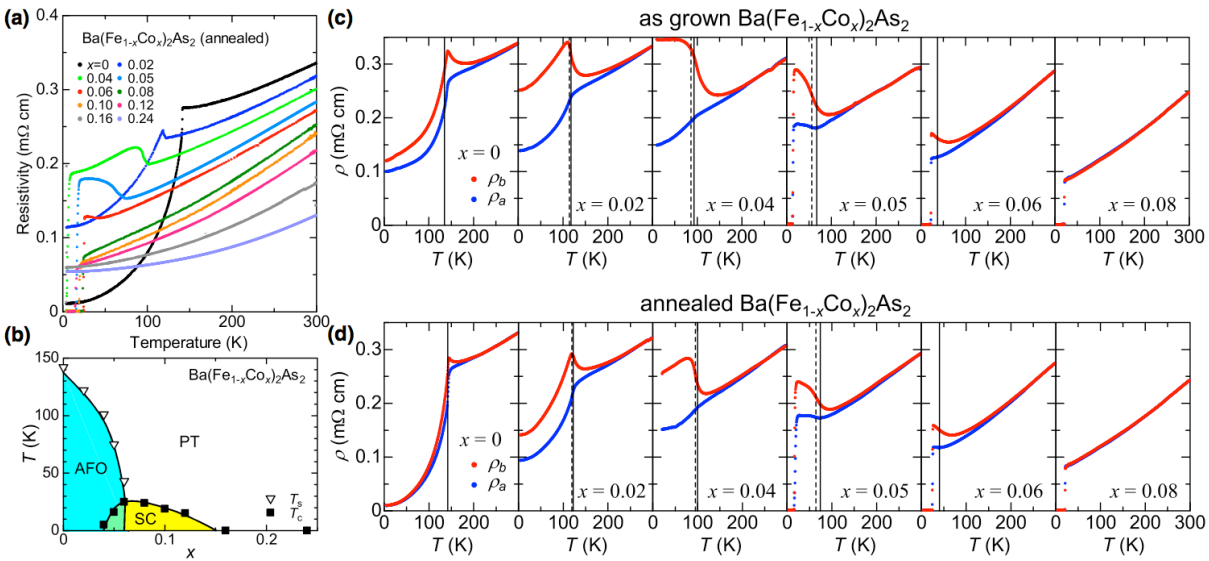
E. P. Rosenthal[1], E. F. Andrade[1], C. J. Arguello[1], R. M. Fernandes[2], L. Y. Xing[3], X. C. Wang[3], C. Q. Jin[3], A. J. Millis[1], A. N. Pasupathy[1]




E. Rosenthal *et al*, 1307.3526

# Anisotropy of the In-Plane Resistivity of Underdoped $Ba(Fe_{1-x}Co_x)_2As_2$ Superconductors Induced by Impurity Scattering in the Antiferromagnetic Orthorhombic Phase

S. Ishida,[1,2,3] M. Nakajima,[1,2,3] T. Liang,[1,2,3] K. Kihou,[2,3] C. H. Lee,[2,3] A. Iyo,[2,3] H. Eisaki,[2,3] T. Kakeshita,[1,3] Y. Tomioka,[2,3] T. Ito,[2,3] and S. Uchida[1,3]



# Anisotropy of the In-Plane Resistivity of Underdoped $Ba(Fe_{1-x}Co_x)_2As_2$ Superconductors Induced by Impurity Scattering in the Antiferromagnetic Orthorhombic Phase

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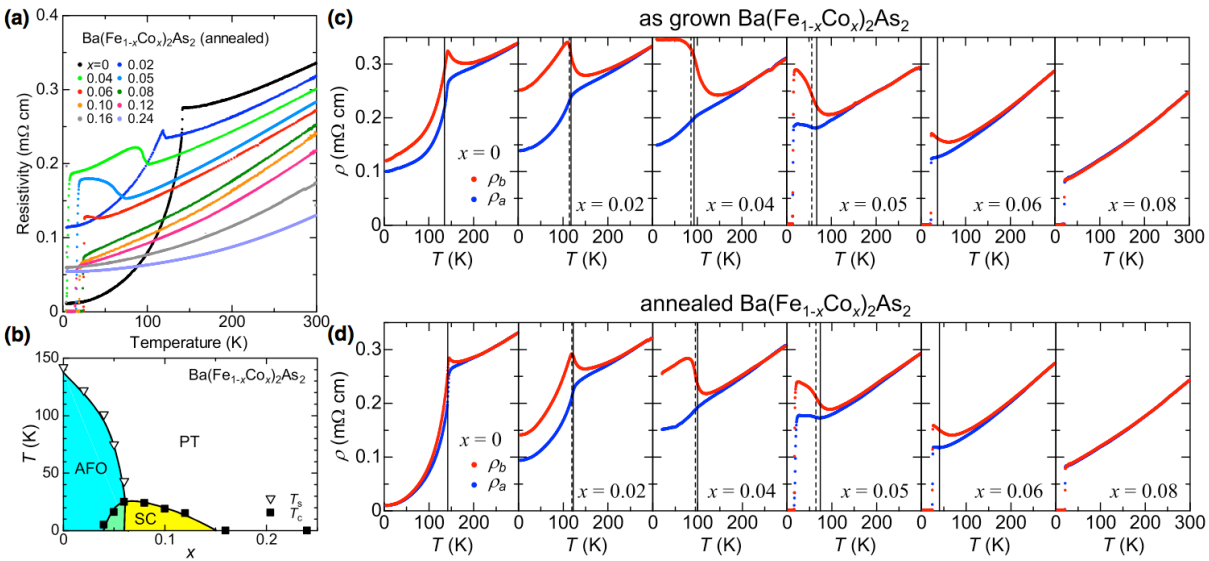


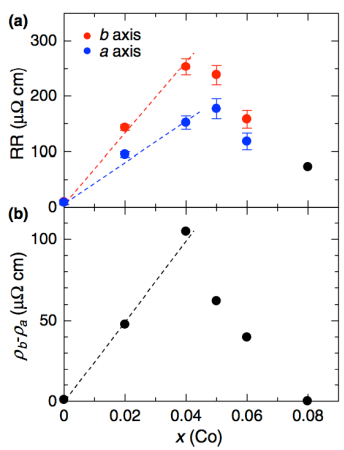


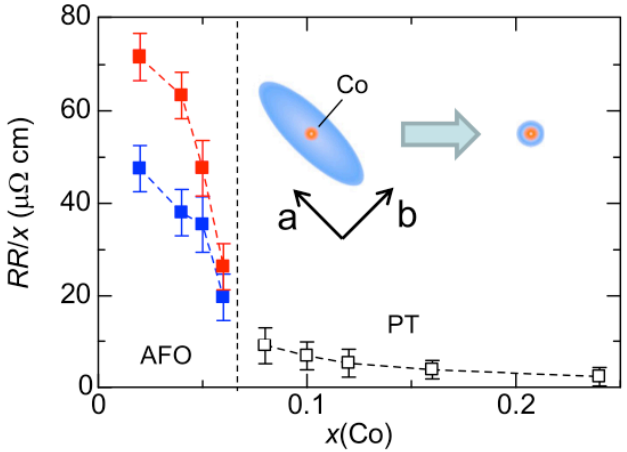

PRL 110, 207001 (2013) PHYSICAL REVIEW LETTERS week ending 17 MAY 2013

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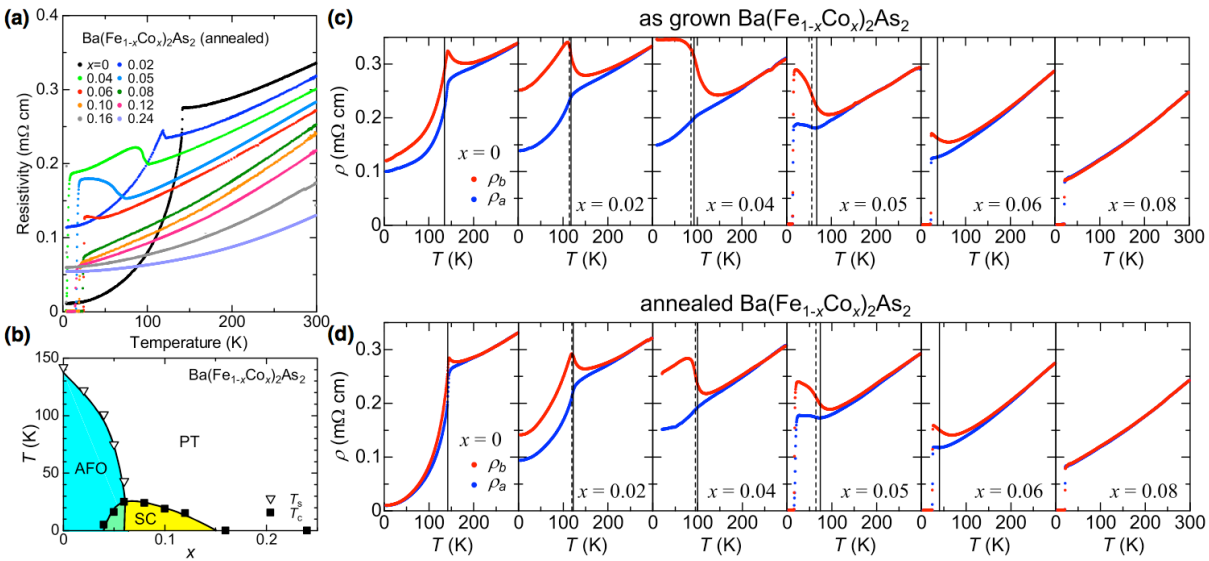
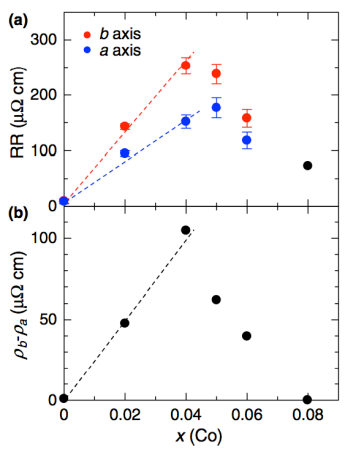
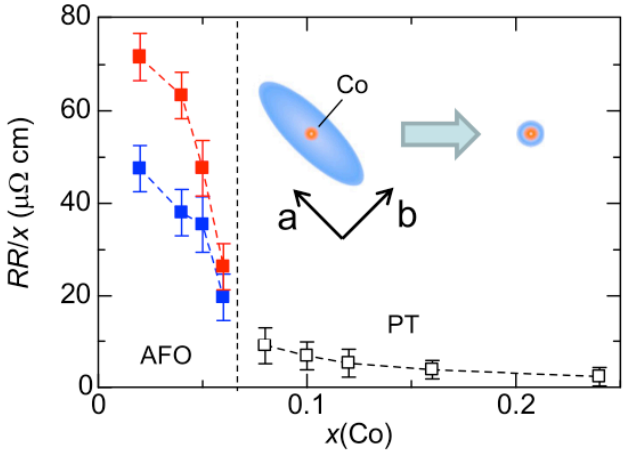



Impurity- induced resistivity anisotropy



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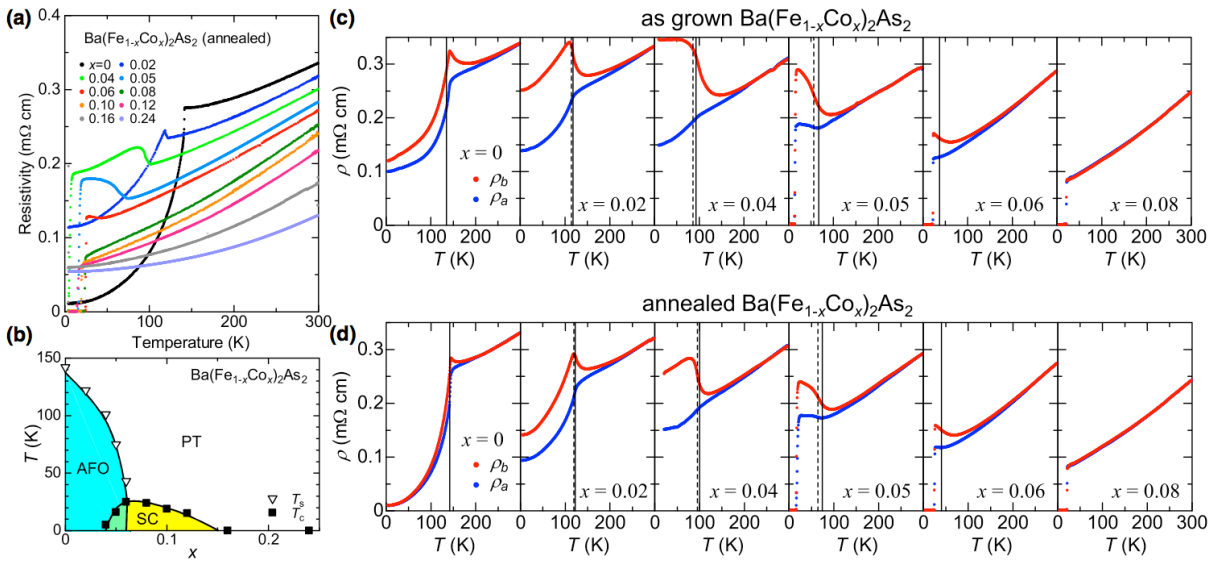
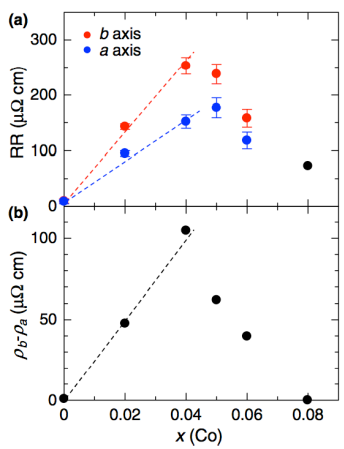
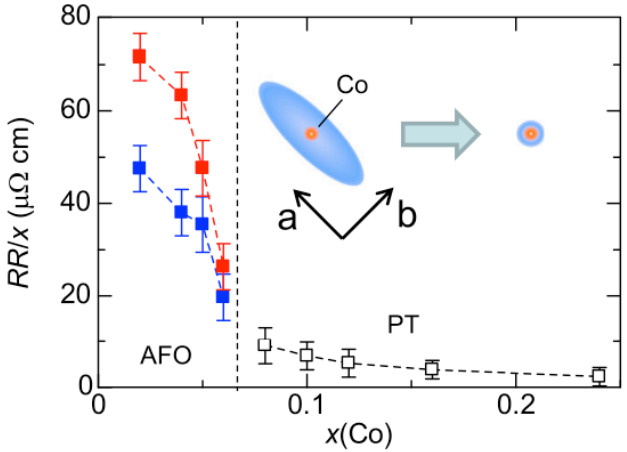
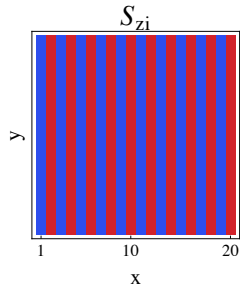



Much smaller resistivity anisotropy of hole-doped $Ba_{1-x}K_xFe_2As_2$

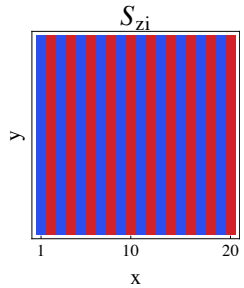


# What do point-like impurities actually do in the SDW phase?



They generate new emergent elongated impurity states!



# Origin of electronic dimers in the SDW phase

$$H = H_0 + H_{int} + H_{imp};$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t_{\mathbf{ij}}^{\mu\nu} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}$$

$$\begin{aligned} H_{int} = U \sum_{\mathbf{i},\mu} n_{\mathbf{i}\mu\uparrow} n_{\mathbf{i}\mu\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\mu<\nu,\sigma\sigma'} n_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\nu\sigma'} \\ - 2J \sum_{\mathbf{i},\mu<\nu} \vec{S}_{\mathbf{i}\mu} \cdot \vec{S}_{\mathbf{i}\nu} + J' \sum_{\mathbf{i},\mu<\nu,\sigma} c_{\mathbf{i}\mu\sigma}^{\dagger} c_{\mathbf{i}\mu\bar{\sigma}}^{\dagger} c_{\mathbf{i}\nu\bar{\sigma}} c_{\mathbf{i}\nu\sigma}, \end{aligned} \tag{3}$$

$$H_{imp} = V_{imp} \sum_{\mu\sigma} c_{\mathbf{i}^*\mu\sigma}^{\dagger} c_{\mathbf{i}^*\mu\sigma}$$

# Origin of electronic dimers in the SDW phase

$$H = H_0 + H_{int} + H_{imp};$$

$$H_0 = \sum_{\mathbf{ij},\mu\nu,\sigma} t^{\mu\nu}_{\mathbf{ij}} c^{\dagger}_{\mathbf{i}\mu\sigma} c_{\mathbf{j}\nu\sigma} - \mu_0 \sum_{\mathbf{i}\mu\sigma} n_{\mathbf{i}\mu.\sigma}$$

$$H^{\mu\nu}_{\mathbf{ij}\sigma} = t^{\mu\nu}_{\mathbf{ij}} + \delta_{\mathbf{ij}}\delta_{\mu\nu}[-\mu_0 + \delta_{\mathbf{ii}^*} V_{imp} + U\langle n_{\mathbf{i}\mu\bar{\sigma}}\rangle + \sum_{\mu'\neq\mu} (U'\langle n_{\mathbf{i}\mu'\bar{\sigma}}\rangle + (U'-J)\langle n_{\mathbf{i}\mu'\sigma}\rangle)],$$

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

# Origin of electronic dimers in the SDW phase

$$H = H_0 + H_{int} + H_{imp};$$

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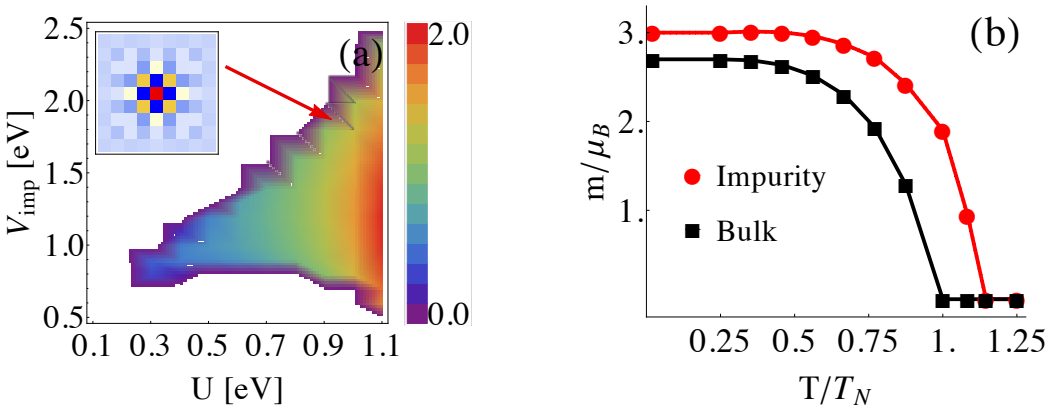
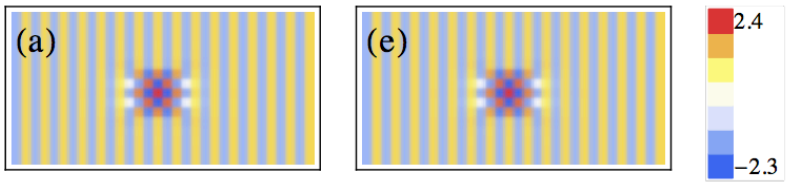
$$H_{imp} = V_{imp} \sum_{\mu\sigma} c^{\dagger}_{\mathbf{i}*\mu\sigma} c_{\mathbf{i}*\mu\sigma}$$

T=0



# Origin of electronic dimers in the SDW phase



# Origin of electronic dimers in the SDW phase

Nematogens:

1) robust (not sensitive to band, V_imp ..)

2) cooling-dependent!

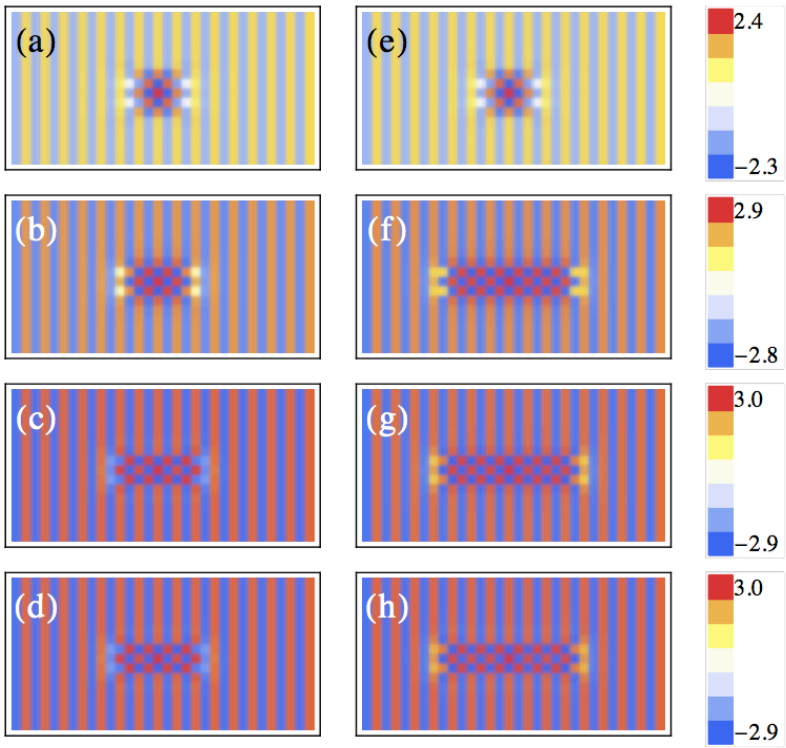



FIG. 2. (Color online) Magnetization in real-space upon lowering $T$ with $U = 1.6$eV and $V_{imp} = 0.1$eV. From top to bottom: $T/T_N = 0.88, 0.67, 0.46, 0.25$. At each $T$, the system is iterated until the bulk magnetization has converged. The

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# Origin of electronic dimers in the SDW phase

magnetization

density

LDOS

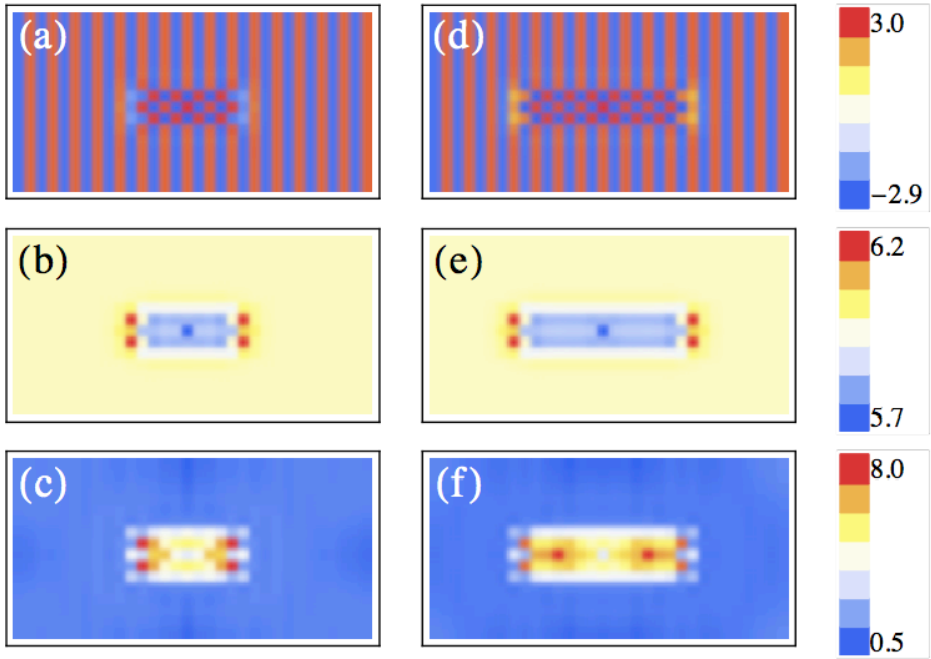


FIG. 3. (Color online) 2D real-space maps of (a,d) the magnetization, (b,e) the total electron charge density, and (c,f) the low-energy integrated LDOS for the same two low-$T$ nematogens shown in Fig. 2(d,h).

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# Origin of electronic dimers in the SDW phase

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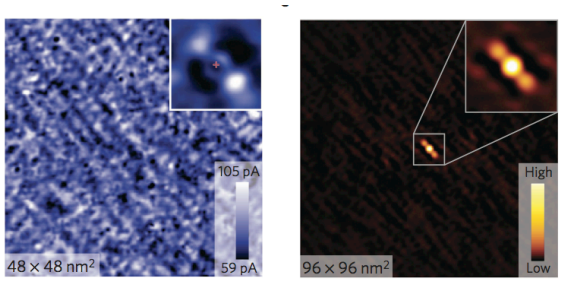


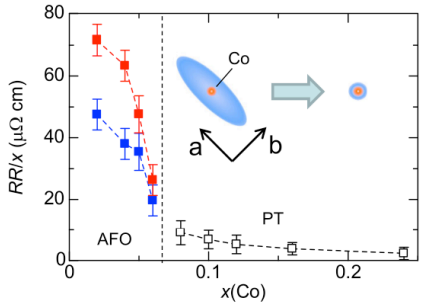


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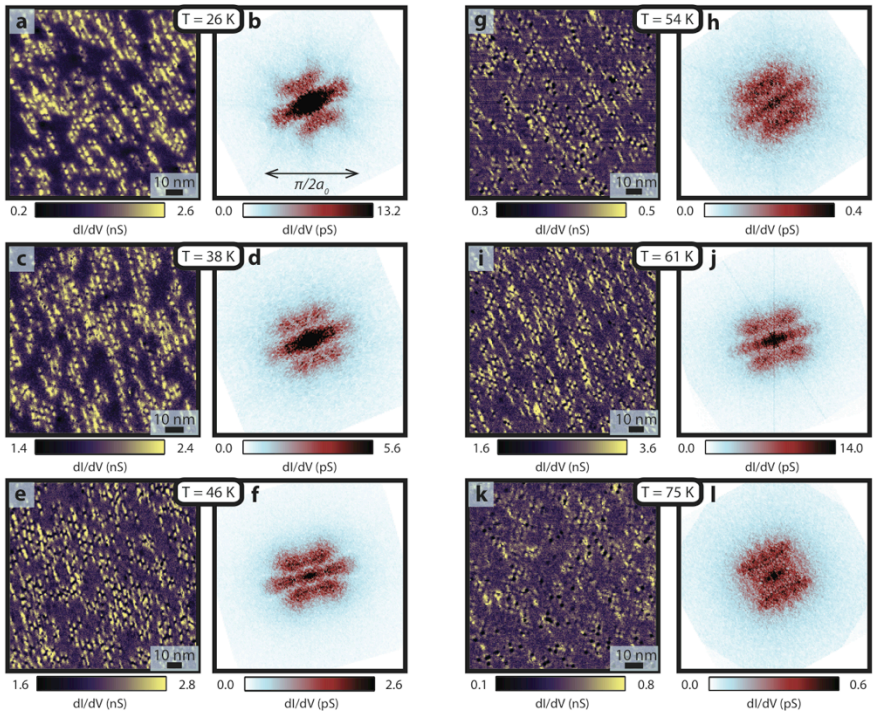


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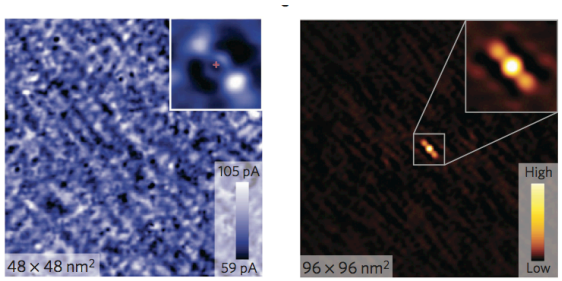


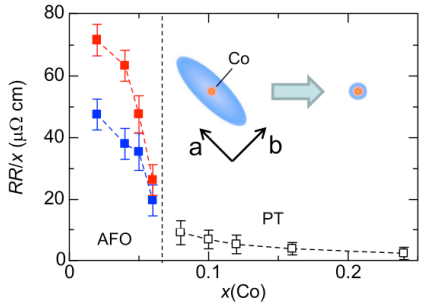


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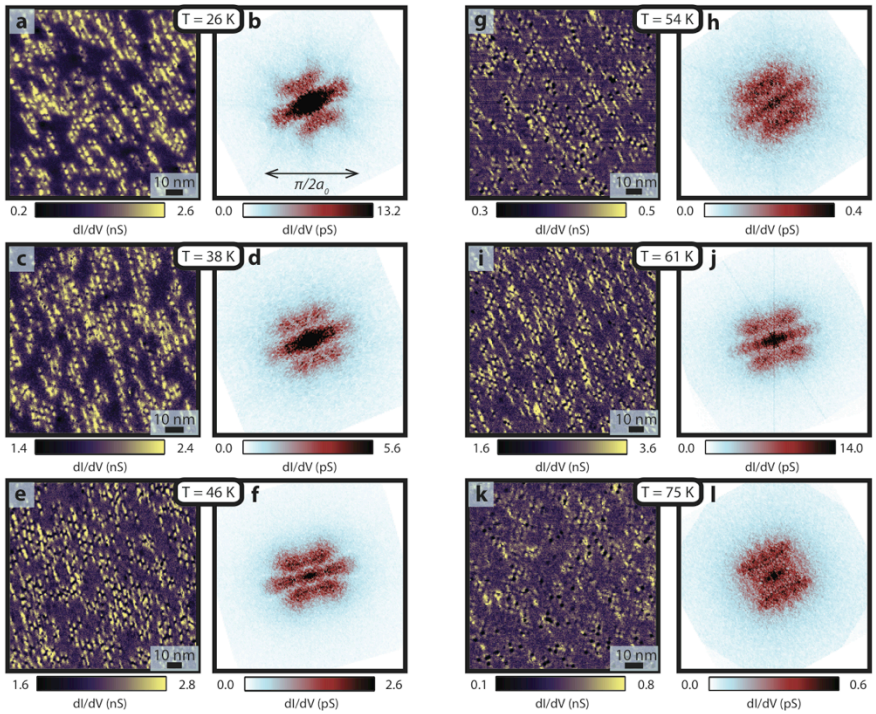


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We now have a microscopic candidate for these dimers

# Origin of electronic dimers in the SDW phase

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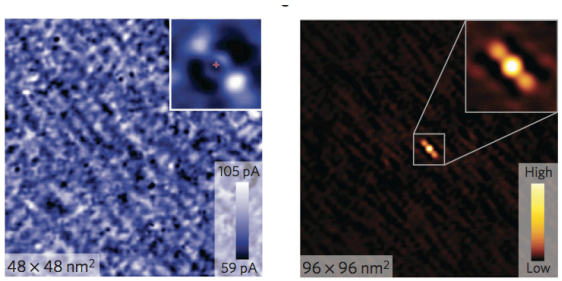


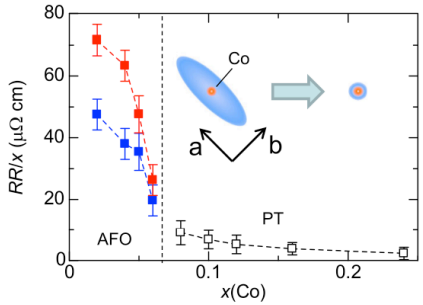


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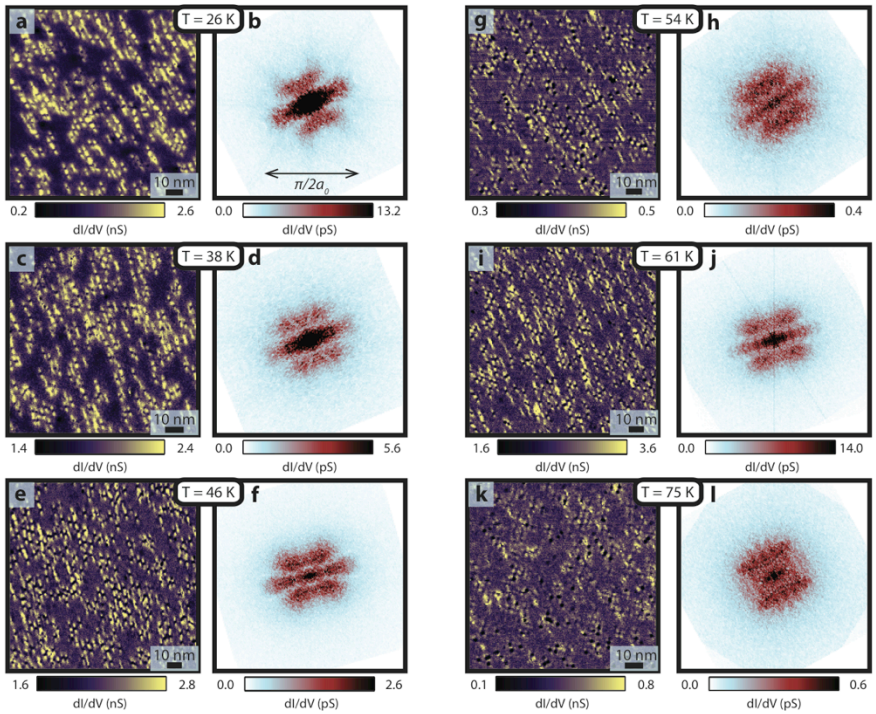
$T_N$=39K

$T_S$=54K

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Open question: how can the electronic dimers survive above $T_S$?

# Conclusions

## Disorder in superconductors:

- rich bound state scenario (nonmagnetic, magnetic, induced order).

- more work needed for understanding of all details.

## Disorder in the SDW phase:

- nonmagnetic point-like potentials generate large 1D emergent nematogens.

- the nematogens constitute a microscopic candidate for electronic dimers seen by STM and the impurity-induced transport anisotropy.

Thank you for your attention