Magnetic effects of strain induced dislocation in unconventional superconductors

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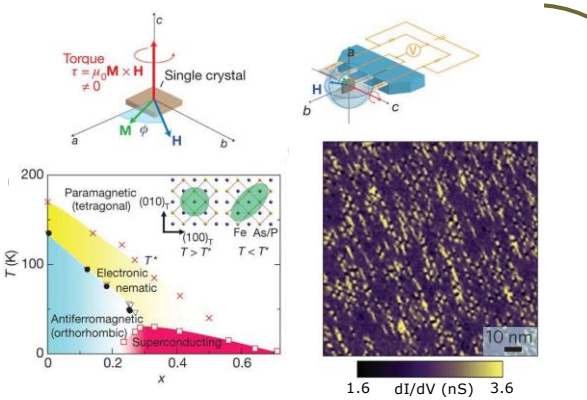
Motivation



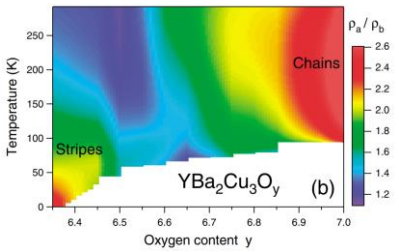
$BaFe_2(As_{1-x}P_x)_2$

Kasahara et al., Nature 486, 382 (2012)

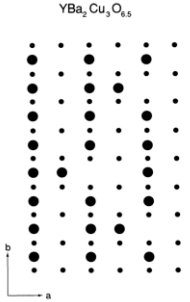
NaFeAs

Rosenthal et al., Nat Phys 10, 225 (2014)

- A nematic magnetic response in torque magnetometry observed in $BaFe_2(As_{1-x}P_x)_2$ above global structural transition temperature
- Meta-nematic transition proposed in the article but could be strain-driven nematicity!
- Observed linear defects in NaFeAs tunneling study, robust up to temperatures significantly higher than T_s.



Ando et al.,PRL 88, 137005 (2002)

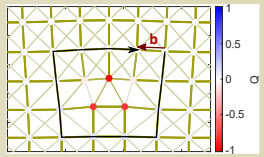


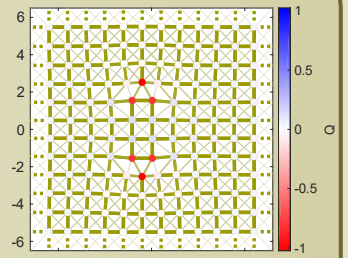
Veal et al., PRB 42, 6305 (1990)

- Anisotropy at high oxygen content due to Cu-O-Cu chains
- Anisotropy at low oxygen content might be result of increased correlation in presence of remnant chain fragments which are dislocation-like linear defect structures

Dislocation geometry

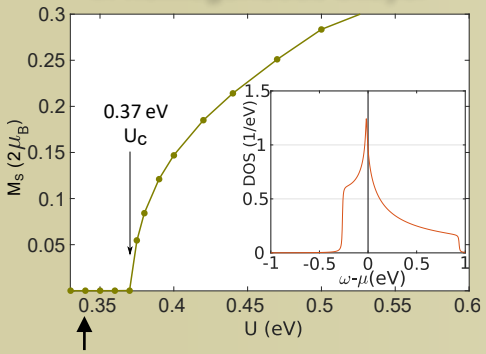
- Can host interstitial atoms inducing local charge accumulation and modify band structure
- A solitary edge-dislocation in a lattice has non-zero Burgers vector **b**
- Burgers vector for a dislocation anti-dislocation pair vanishes far away in the system





- Simulated with Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)
- Modified hopping via interpolation and overlapping atomic orbitals
- Accumulated charges via valence bond sum

Critical Hubbard repulsion in homogeneous bilayer



Dislocation studied at U = 0.34 eV

Bilayer Hamiltonian (spin rotationally invariant)

$$H = H_{tb} + H_{tb}^{\perp} + H_Q + H_{SO} + H_U + H_B$$

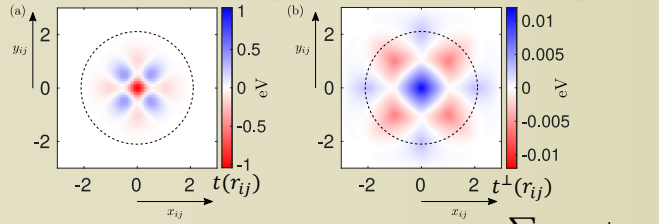
$$H_Q = \sum_{i,\sigma} V_{eff}\, Q_i c_{i,\sigma}^{\dagger} c_{i,\sigma}$$

$$Q_i = Q_{Cu} + A \sum_{|r_{ij}|<1.3} Q_O \exp\left(-|r_{ij}|^2/\lambda^2\right)$$

$$H_{SO} = (-1)^{\nu}\gamma\left\{\sum_{\langle i,j_y\rangle} i\left(c_{i,\uparrow}^{\dagger}c_{j_y,\downarrow} - c_{j_y,\uparrow}^{\dagger}c_{i,\downarrow}\right) + \sum_{\langle i,j_y\rangle}\left(c_{i,\uparrow}^{\dagger}c_{j_x,\downarrow} - c_{j_x,\uparrow}^{\dagger}c_{i,\downarrow}\right)\right\} + h.c.$$

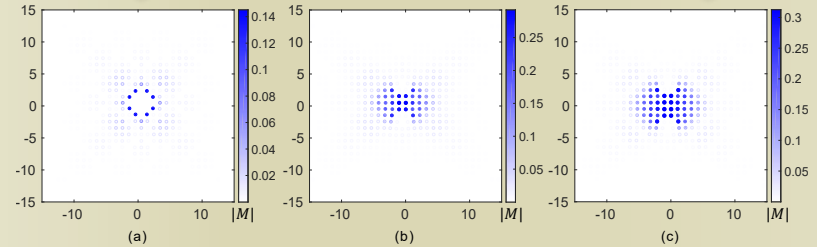
H_Q and H_{SO} crucial in driving the anisotropy

Intra-layer hopping Inter-layer hopping

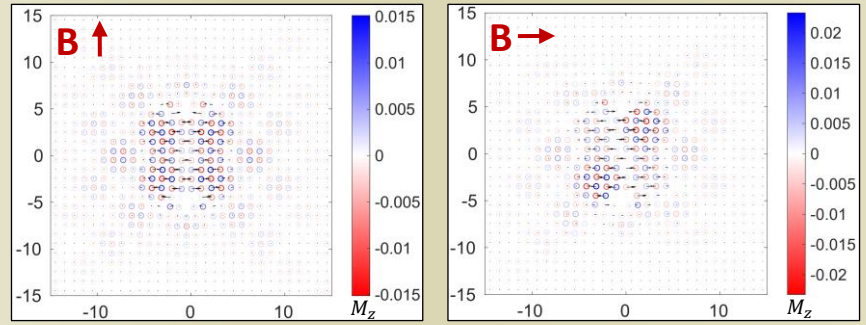


Continuous hopping maps in a distorted lattice: $H_{tb} = \sum_{i,j,\sigma} t(r_{ij})\, c_{i,\sigma}^{\dagger} c_{j,\sigma}$

Magnetization evolution with dislocation length



Magnetic response in Zeeman field



Energy difference in the configuration estimates to same order of magnitude torque in magnetometry experiments

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