Emergent Defect States in Fe-based Superconductors

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Introduction

Stong local breaking of C_4 symmetry by defects in tetragonal or nearly tetragonal Fe-based superconductors has been reported by many scanning tunneling microscopy (STM) groups. In some cases this is in the magnetic state which tends to have $(\pi,0)$ order which already breaks C4[1], but sometimes this occurs in nonmagnetic systems as well[2]. A remarkable aspect of the electronic states created by an atomic scale defect is that they tend to be highly elongated, with lengths up to 16 unit cells in FeSe. Furthermore, they have a dimerlike structure, with the local density of states (LDOS) or charge peaked at the ends of the "nematogen" There has been no theoretical understanding of the origin of these defect states.

Results and Discussion

We performed Bogoliubov-de Gennes (BdG) calculations of simple δ-function defects to simulate impurities in the spin density wave (SDW) state of Fe-based superconductors, including Hubbard and Hund's rule couplings treated in mean field. As expected, the impurities nucleated droplets of distorted magnetic order for sufficiently large correlation strength. The surprise was that the local magnetism was of (π, π) type, that the structures are highly elongated, and that dimers indeed form at the ends of the nematogens.

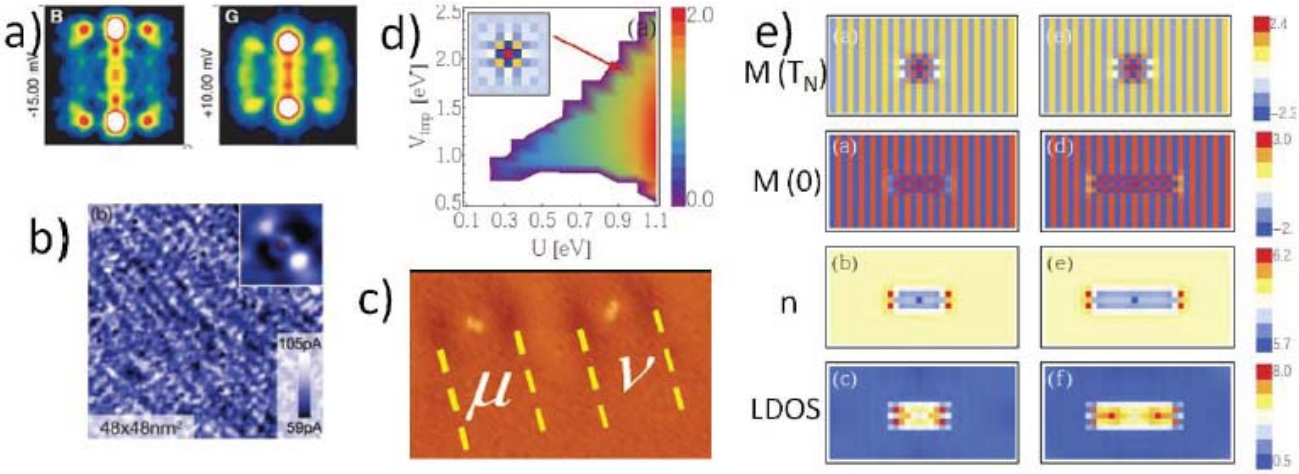

Fig. 1 a) Two-fold quasiparticle interference signature observed by Cornell group on surface of Ca-122 parent compound[1];b) Real space image in current map I(r) of electronic dimer near Co dopant in Ca-122[2]; c) Emergent defect state in nonmagnetic FeSe[3] showing 16 unit cell ``electronic dimers'' (dark areas)spanning local ``geometric dimers'' aligned with nearest neighbor Se atoms nearimpurity, registered with Fe site. d) Region of stability for orbital diagonal impurity potential V_{imp} vs. Coulomb interaction U in inhomogeneous Hartree-Fock diagonalization of Hubbard Hund model from Ref. 4. e) Results for V_{imp} =0.1, U=1.6eV, J=U/4 for two different cooling rates fast (left) and slow (right). Top row: magnetization M in normal state; next: magnetization M at T=0; next: charge distribution n; bottom row: LDOS integrated from -40 meV to 0 meV.

Conclusions

We believe that simple defects in systems with strong $(\pi,0)$ order or fluctuations have a natural tendency to nucleate long dimerlike electronic nematogens, due to the proximate low-lying (π,π) magnetic order, and the system's desire to minimize its energy by creating as uniform a charge and magnetic state as possible, including a long unfrustrated boundary of the two magnetic states.

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