**Theoretical Visualization of STM Images in Inhomogeneous Superconductors**

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**Introduction**

Theoretical calculations of STM images on cuprate superconductors have been confined almost exclusively to models of electrons hopping on a square lattice corresponding to the Cu sites in the CuO2 plane; this is a clear disadvantage, for example when the elusive charge order is seen to correspond to local density of states modulations primarily on the O sites.



Calculation of Zn impurity in BSCCO-2212: a) traditional Bogoliubov-de Gennes (BdG) solution; (b) BdG+W [1] approach; (c) experiment from Ref. [2].



Quasiparticle interference patterns Fouier transformed density of states (**q**,) for =24meV for weak scattererer: (a) BdG; (b) BdG+W; [2] (c) experiment from Ref. [3].

**Results and Discussion**

We developed a method [1,4] that started with the lattice calculations that we and others had already performed, and simply used the Wannier functions generated in the process of downfolding a renormalized DFT band structure onto a tight-binding model to calculate the continuum instead of the lattice Green’s function.

**Conclusions**

The crucial aspect was found to be the tails of the Cu Wannier functions, which include significant weight on apical O sites in neighboring unit cells. The results compare nearly perfectly to experimental findings that have puzzled the community for more than 10 years.

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**References**

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[2] S. Pan et al, Nature **403**, 746 (2000).

[3] K. Fujita et al. Science 344, 612 (2014).