Structure of Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ Super modulation from ab initio Calculations

Y. He, S. Graser, P.J. Hirschfeld and H.-P. Cheng (UF, Physics)

Introduction
Recent scanning tunneling spectroscopy experiments on Bi-2212 where O dopant positions were directly imaged [1] have stimulated a good deal of work on the effects of dopants on the physics of the CuO$_2$ plane. The observed correlations between dopant positions and the local gap size, along with many other correlations, suggests that the dopants modulate the BCS pair interaction in the material locally[2]. This suggests the possibility of a new paradigm for investigating pairing and its origins in the cuprates. Measurements tell us how the gap responds to a spatial perturbation on the atomic scale. Density functional theory (DFT) or x-ray analysis can then help determine the exact atomic displacements which occur. With this information in hand, one can use it to calculate local changes in electronic structure and constrain pairing theories of high-temperature superconductors. Very recently, the Cornell STM group has measured a 10% variation of the superconducting gap directly correlated with the phase of the structural supermodulation known to exist in BSSCO-2212 [3] which were shown to be entirely consistent with the magnitude of the pairing interaction modulations expected from the dopant work [4].

Results and Discussion
Results of a DFT structural calculation involving 5x2 complete BSCCO-2212 unit cells[5] are in excellent agreement with those of x-ray analyses, as shown, e.g. in 2nd panel of Figure, where structure of modulated Bi-2212 (nominal crystal structure shown on left) as found by DFT (top center) and x-ray diffraction (bottom center) are compared. Furthermore the atomic displacements found correlated in exactly the same way with increased pairing strength as in the impurity problem!

Conclusions
The most important effect on the CuO$_2$ plane of both the structural supermodulation and the O dopant appears to be the tilting of the CuO$_2$ half-octahedra and concomitant buckling of the plane; this corresponds locally to increased superconducting gap. The local electronic structure from these calculations will now be downfolded and the effect on the pair interaction within various models will now be determined.

Acknowledgements
Supported by DE-FG02-05ER46236.

References