Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Local Electronic Structure of Bi2Sr2CaCu2O8 near Oxygen Dopants: A Window on the High-Tc Pairing Mechanism[1] YAO HE, PETER HIRSCHFELD, HAI-PING CHENG, University of Florida — The cuprate material Bi2Sr2CaCu2O8(BSCCO-2212) is believed to be doped by a combination of cation switching and excess oxygen. The interstitial oxygen dopants are of particular interest because scanning tunneling microscopy (STM) experiments have shown that they are positively correlated with the local value of the superconducting gap, and calculations suggest that the fundamental attraction between electrons is modulated locally. In this work, we use density functional theory to try to ascertain which locations in the crystal are energetically most favorable for the O dopant atoms, and how the surrounding cage of atoms deforms. Our results provide support for the identification of STM resonances at -1.0 eV with dopant interstitial O atoms, and show how the local electronic structure is modified nearby.

[1]Supported by DOE under DE-FG02-97ER45660DE-FG02-02ER45995, NSF/DMR/ITR/DMR-032553, ONR/N00014-04-0060, and DOE/DEFG02-05ER46236

Hai-Ping Cheng
University of Florida

Date submitted: 20 Nov 2006 Electronic form version 1.4