MAR11-2010-005511

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

First-principles studies for understanding diverse high-T_c[1]

HAI-PING CHENG, University of Florida

In this talk, I survey results and insights gained from first-principles calculations on materials that exhibit superconducting behavior at temperatures higher than those characteristic of conventional BCS superconductors. These range from highly correlated cuprate Mott insulators as represented by the bismuth-strontium-calcium-copper-oxides (BSCCOs) to border-line itinerant-Mott systems such as the recently discovered 1111 and 122 pnictides. ultimate goal of our studies is to correlate T_c with specific material composition using detailed first-principles calculations in conjunction with many-body physics techniques via the critical step of constructing real-materials model Hamiltonians. By manipulating impurity doping, which plays a crucial role in the phase diagrams of high T_c materials, we hope to find guidance for designing candidate systems with T_c higher than ones currently known. BSCCO material, density functional calculations using a good generalized-gradient approximation (GGA) yield structural information that is correlated to the experimentally observed (STM) super-modulation and impurity peak in the high energy regime ($\sim$1 eV), even though the Kohn-Sham bands from such functionals fail to have a band gap. For FeAs-based high-T_c systems, DFT band-structure calculations provide a very good starting point for constructing model Hamiltonians for studies of spin fluctuation and electron pairing mechanisms. Fermi sheets that have been constructed using Wannier transformed Kohn-Sham states have provided critical information for understanding this family of superconducting materials. Analysis of the details of magnetic ordering, density of states, and 2D vs. 3D features in both the 1111 and 122 materials have been valuable in understanding sometimes perplexing experimental findings. Effects of Co impurities have been studied and fully analyzed as well., I will discuss persistent challenges related to calculations on the structure of the non-magnetic state $Ba_1Fe_2As_2$ system. Both further examination of the underlying physics and development of new approximate functionals are needed.

[1]Supported by DOE/BES and NSF/DMR, computed at NERSC and UF/HPC.