center for nanophysics and advanced materials

Condensed Matter Colloquium

Thursday, February 10, 2011

2 pm, Room 1201

Taner Yildirim

NIST Center for Neutron Scattering

First-principles investigation of recent novel superconductors: Fe-pnictides and K-doped Picene

In this talk, I will present a brief review of our first principles studies on two recent novel superconductors; namely Fe-pnictides (i.e., $BaFe_2As_2$, KFe_2Se_2) and K-doped hydrocarbon Picene, two totally different systems. For iron-based superconductors, our results clearly show that the Fe-spin is the key factor controlling many physical properties of the pnictide systems, including atomic positions, crystal cell size, structural phase transitions, and lattice vibrations and which provides a strong clue about the superconducting mechanism. In particular, we show that there are strong and competing magnetic interactions in these systems that explain both the observed spin-pattern and the structural phase transition. In particular, we present some new results concerning the spin-resolved electron-phonon coupling in these systems. In the second part of the talk, I will discuss a long-standing question, namely "Can simple hydrocarbon molecular solids superconduct?" Unlike many well established high temperature (T_c) superconductors such as cuprates, M_3C_{60}, MgB_2 and iron-pnictides, the possibility of superconductivity in molecular hydrocarbon solids remains a controversial issue. This topic became active again by a recent study reporting superconductivity up to T_c ~17 K in potassium doped Picene [Mitsuhashi et al. Nature, 464,76], a wide-bandgap semiconducting solid hydrocarbon. However, there is no theoretical study about possible mechanism of superconductivity. Here, we will present a detailed first-principles study of the electron-phonon (el-ph) coupling in doped organic molecular solids. As a comparison, we have also studied the el-ph coupling in alkali-doped Pentacene, a similar well-studied hydrocarbon in which no superconductivity has been observed. We discuss the effect of charge transfer as well as pressure on T_c for solid Picene and make predictions for future possible experiments.

Refreshments at 1:30 pm in Room 1305F

physics
University of Maryland