FeAs superconductors: Electronic Structure Calculations are Relevant!

B. N. Harmon and Y. Lee

Ames Laboratory, U.S. Department of Energy, and Iowa State University

In contrast to the early (and continuing) frustrations encountered with the cuprates, electronic structure calculations are providing key insights for the new FeAs based superconductors. This talk will emphasize the remarkable interactions (both static and dynamic) between the magnetism and the lattice. For example, calculations for the collapsed tetragonal phase of $Ca_2Fe_2As_2$ predicted the disappearance of the magnetic moment on the iron sites, which was later confirmed by scattering experiments. For these materials, calculations generally show good agreement with Fermi surface geometries. When photoemission data for LaFeAsO revealed Fermi surface dimensions larger than predicted from the bulk calculations, supercell calculations for the surface states quantitatively agreed with the much larger calipers observed. The lattice coupling with the magnetic moments (antiferromagnetically aligned on the Fe sites) is dramatically demonstrated by first principles calculations of the phonon dispersion curves. Even at room temperature, well above the magnetic ordering temperature, the measured phonon dispersion curves agree much better with the spin polarized calculations. This is an indication of magnetic moments with short-range antiferromagnetic correlations persisting to high temperatures; a phenomena confirmed by neutron scattering measurements.