MAR13-2012-000395

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Ab initio calculations and crystal symmetry considerations for novel FeSe-based superconductors

IGOR MAZIN, NRL

Density functional calculations disagree with the ARPES measurements on both $K_{0.3}Fe_2Se_2$ superconducting phase and $FeSe/SrTiO_3$ monolayers. Yet they can still be dramatically useful for the reason that they respect full crystallographic symmetry and take good account of electron-ion interaction. Using just symmetry analysis, it is shown that nodeless d-wave superconductivity is not an option in these systems, and a microscopic framework is derived that leads to a novel s-wave sign-reversal state, qualitatively different from the already familiar $s_{\pm}$ state in pnictides and bulk binary selenides. Regarding the FeSe monolayer, bonding and charge transfer between the film and the substrate is analyzed and it is shown that the former is weak and the latter negligible, which sets important restrictions on possible mechanisms of doping and superconductivity in these monolayers. In particular, the role of the so-called "Se etching," necessary for superconductivity in FeSe monolayers, is analyzed in terms of electronic structure and bonding with the substrate.