MAR16-2015-002686

Abstract for an Invited Paper
for the MAR16 Meeting of
the American Physical Society

**Origin of superconductivity in $KFe_2As_2$ under positive and negative pressures and relation to other Fe-based families**[1]

ROSER VALENTI, Institute of Theoretical Physics, University of Frankfurt

$KFe_2As_2$ shows an intricate behavior as a function of pressure. At ambient pressure the system is superconductor with a low critical temperature $T_c$=3.4 K and follows a V-shaped pressure dependence of $T_c$ for moderate pressures with a local minimum at a pressure of 1.5 GPa. Under high pressures $P_c$=15 GPa, $KFe_2As_2$ exhibits a structural phase transition from a tetragonal to a collapsed tetragonal phase accompanied by a boost of the superconducting critical temperature up to 12 K. On the other hand, *negative* pressures realized through substitution of K by Cs or Rb decrease $T_c$ down to 2.25K. In this talk we will discuss recent progress on the understanding of the microscopic origin of this pressure-dependent behavior by considering a combination of ab initio density functional theory with dynamical mean field theory and spin fluctuation theory calculations [1-3]. We will argue that a Lifshitz transition associated with the structural collapse changes the pairing symmetry from $d$-wave (tetragonal) to $s_\pm$ (collapsed tetragonal) at high pressures while at ambient and negative pressures correlation effects appear to be detrimental for superconductivity. Further, we shall establish cross-links to the chalcogenide family, in particular FeSe under pressure [4]. [1] S. Backes, D. Guterding, H. O. Jeschke, R. Valenti, New J. Phys. 16, 083025 (2014). [2] D. Guterding, S. Backes, H. O. Jeschke, R. Valenti, Phys. Rev. B 91, 140503(R) (2015). [3] S. Backes, H. O. Jeschke, R. Valenti, Phys. Rev. B (in press). [4] J. K. Glasbrenner, I. I. Mazin, H. O. Jeschke, P. J. Hirschfeld, R. Valenti Nature Physics 11, 953 (2015).

[1]The Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged for financial support.