Study of local structural distortions in Ba$_{1-x}$K$_x$Fe$_2$As$_2$ superconductors

E. BOZIN, C. FARROW, J. LIU, Y. SHANG, Columbia University, R. CORTES-GIL, S. CLARKE, University of Oxford, J. HILL, S. BILLINGE, Brookhaven National Laboratory — In iron pnictides [1] presence of orbital degrees of freedom on the Fe site is one of the notable differences from cuprate superconductors (SC). The presence of an electron in a particular orbital directly influences the positions of the nearest neighbor ions and couples strongly to the lattice. The orbital degrees of freedom potentially strongly enhance the electron-phonon coupling, and could play a central role in the SC pairing mechanism. Understanding how this orbital occupancy evolves as a function of doping and temperature is of crucial importance. Probing orbital occupancy directly is difficult as the orbital order is expected to be ferro (identical from site to site), and thus not amenable to conventional scattering experiments. Doping towards the SC state destroys long range magnetic order, but the presence of short range ferro-orbital order is suspected. Results will be presented of a systematic x-ray total scattering based atomic pair distribution function study, to map out the local structure across the phase diagram of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ [2], and investigate the importance of the orbital degree of freedom in this new class of materials. [1] Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008). [2] Y.J. Uemura, Nature Materials 8, 253 (2009). Supported by the DOE under Contract. No. DE-AC02-98CH10886.

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Date submitted: 07 Dec 2009       Electronic form version 1.4