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Local

Atomic and Electronic Structure of $K_{0.8}Fe_{1.6+x}Se_2$: Structural Order and Disorder TREVOR TYSON, TIAN YU, New Jersey Institute of Technology, SU JUNG HAN, Brookhaven National Laboratory, MARK CROFT, Rutgers University, GENDA D. GU, IVO DIMITROV, QIANG LI, Brookhaven National Laboratory — The local structure of superconducting single crystals of $K_{0.8}Fe_{1.6+x}Se_2$ was studied by x-ray absorption spectroscopy. Near-edge spectra reveal that the average valence of Fe is 2+. The structure about the Se and Fe sites shows a high degree of order in the nearest neighbor Fe-Se bonds. On the other hand, the combined Se and K local structure measurements reveal a very high level of structural disorder in the K layers. The temperature dependence of the Fe-Se atomic correlation follows that of the Fe-As correlation in $LaFeAsO_{0.89}F_{0.11}$. In $K_{0.8}Fe_{1.6+x}Se_2$, the nearest neighbor Fe-Fe bonds has a lower Einstein temperature and higher structural disorder than in $LaFeAsO_{0.89}F_{0.11}$. For higher shells, an enhancement of the second nearest neighbor Fe-Fe interaction is found just below T_c and suggests that correlations between Fe magnetic ion pairs beyond the first neighbor are important in models of magnetic order and superconductivity in these materials. This research is supported by DOE BES Grant DE-FG02-07ER46402 (NJIT) for T.A.T and T.Y. and DOE BES Contract No. DE-AC0298CH10886. (BNL), for S.J.H, G.G, I.K.D, and Q. L.

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