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Defect Structures and nonstoichiometry in the $K_xFe_{2-y}Se_2$ by X-ray diffraction. JOHN CLARIDGE, ALEXEY GANIN, ALEC MCLENNAN, JOHN BACSA, MATTHEW ROSSEINSKY, University of Liverpool, YASUHIRO TAKABAYASHI, KOSMAS PRASSIDES, Durham University — The mechanisms of charge carrier density control in the iron pnictide and chalcogenide superconductors are important as small changes in composition produce metal-insulator transitions and generate superconductivity at temperatures of up to 37K in chalcogenides and 55K in pnictides. All of the reported materials are based on a square FeX (X = Se, As) layer built from edge-sharing of FeX_4 tetrahedra. Insertion of alkali metal cations between FeSe layers affords superconductivity in $A_xFe_{2-y}Se_2$ (A = K, Rb, Cs, Tl: $0.7 < x < 1$, $0 < y < 0.5$) materials highlites the defect chemistry as the iron charge states close to +2 found in the other Fe-based superconductors require the creation of considerable defect concentrations on either or both iron and alkali metal sites. Ordering of the tetrahedral site vacancies in two crystals of refined compositions $K_{0.93(1)}Fe_{1.52(1)}Se_2$ and $K_{0.862(3)}Fe_{1.563(4)}Se_2$ produces a fivefold expansion of the parent $ThCr_2Si_2$ unit cell in the ab plane which can accommodate 20% vacancies on a single site within the square FeSe layer. The iron charge state is maintained close to +2 by coupling of the level of alkali metal and iron vacancies, doping mechanisms, which can operate at both average and local structure levels will be discussed. These structures will also be considered in terms of their local ordering and with relation to other defect chalcogenide layer structures and possible phase segregation.

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