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Electronic structure and magnetism of doped $A_xFe_{2-y}Se_2$ YUAN-YEN TAI, Dept. of Physics, Univ. of Houston, Houston, Texas 77054, USA, JIAN-XIN ZHU, MATTHIAS J. GRAF, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, C.S. TING, Dept. of Physics, Univ. of Houston, Houston, Texas 77054, USA — We develop a new multi-orbital t-J Hamiltonian with realistic tight-binding and Heisenberg parameters to study the electronic and magnetic structure of $A_xFe_{2-y}Se_2$ superconductors for 0<y<0.4. The ARPES experiments are fitted by a tight-binding lattice model with random vacancy order. We find that the vacancy order greatly affects the electronic band structure. For intermediate doping levels $0 < y < 0.4$, the stable electronic structure is a compromise between the solution for y=0 and y=0.4. Based on this model, we study the paramagnetic and antiferromagnetic (AFM) phases of $A_{0.8}Fe_{1.6}Se_2$. In the AFM phase the calculated spin susceptibility for the bare band structure agrees with a block-spin structure. This theoretical result is in good agreement with neutron scattering experiments of the spin structure. Furthermore, we show the results on the evolution of low-energy quasiparticle states with electron filling factor in the vacancy-ordered magnetic state.

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