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Vacancy-driven orbital and magnetic order in (K,Tl,Cs)$_y$Fe$_{2-x}$Se$_2$[1] WEICHENG LV, WEI-CHENG LEE, PHILIP PHILLIPS, Department of Physics, University of Illinois — We investigate the effects of the $\sqrt{5} \times \sqrt{5}$ Fe vacancy ordering on the orbital and magnetic order in (K,Tl,Cs)$_y$Fe$_{2-x}$Se$_2$ using a three-orbital (t_{2g}) tight-binding Hamiltonian with generalized Hubbard interactions. We find that vacancy order enhances electron correlations, resulting in the onset of a block antiferromagnetic phase with large moments at smaller interaction strengths. In addition, vacancy ordering modulates the kinetic energy differently for the three t_{2g} orbitals. This results in a breaking of the degeneracy between the d_{xz} and d_{yz} orbitals on each Fe site, and the onset of orbital order. Consequently, we obtain a novel inverse relation between orbital polarization and the magnetic moment. We predict that a transition from high-spin to low-spin states accompanied by a crossover from orbitally-disordered to orbitally-ordered states will be driven by doping the parent compound with electrons, which can be verified by neutron scattering and soft X-ray measurements.

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