

Mott Transition, Magnetism, and Pairing Symmetry of $(\text{Tl}, \text{K})_y\text{Fe}_x\text{Se}_2$

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The discovery of superconductivity with a $T_c \sim 30\text{K}$ in the new 122 iron-chalcogenides $(\text{Tl}, \text{K})_y\text{Fe}_x\text{Se}_2$, in the vicinity of an antiferromagnetically ordered and insulating state, promises to shed new light on both the role of electronic correlations and nature of magnetism and superconductivity of iron-based superconductors. By studying a multi-orbital Hubbard model using slave-rotor method, we show the band narrowing effects due to vacancy ordering may drive the system to a Mott insulating phase.¹ By studying an extensive J_1 - J_2 model, we further show vacancy ordering may also affects the exchange couplings in the insulating phase and results in exotic antiferromagnetic states.²

To understand the superconductivity in the 122 iron-chalcogenides, we study a multi-orbital $t - J_1 - J_2$ model, and show that an $A_{1g} s_{x^2-y^2}$ state and a $B_{1g} d_{x^2-y^2}$ state are quasi-degenerate in the $J_1 \sim J_2$ magnetic frustration regime. We find the pairing amplitudes are of the same order as their pnictides counterparts, making it natural that the maximum T_c is comparable in the two systems.³

¹R. Yu, J.-X. Zhu, and Q. Si, arXiv:1101.3307, to appear in PRL.

²R. Yu, P. Goswami, and Q. Si, arXiv:1104.1445.

³R. Yu, P. Goswami, Q. Si, P. Nikolic, and J.-X. Zhu, arXiv:1103.3259.