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Magnetic state of $K_{0.8}Fe_{1.6}Se_2$ from a five-orbital Hubbard model in the Hartree-Fock approximation¹ QIN-LONG LUO, ANDREW NICHOLSON, ADRIANA MOREO, ELBIO DAGOTTO, Univ. of Tennessee/ORNL, JOSÉ RIERA, Universidad Nacional de Rosario, DAO-XIN YAO, Sun Yat-Sen Univ. — The fiveorbital Hubbard model (without lattice distortions) is investigated to study theoretically the recently discovered Fe-based superconductors $K_{0.8}$ Fe_{1.6}Se₂, by using the real-space Hartree-Fock approximation and employing a 10×10 Fe cluster with Fe vacancies in a $\sqrt{5} \times \sqrt{5}$ pattern[1]. The phase diagram contains an insulating state with the same spin pattern as observed experimentally, involving 2×2 ferromagnetic plaquettes coupled with one another antiferromagnetically. The magnetic moment $\sim 3\mu_B/\text{Fe}$ is in good agreement with experiments. Several other competing phases are also stabilized in the phase diagram, in agreement with recent calculations using phenomenological models. [1] Qinlong Luo et al., Phys. Rev. B 84, 140506(R) (2011), and references therein.

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