

Abstract Submitted
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Novel Magnetism in $K_{0.8}Fe_{1.6}Se_2$ Explained in the Unified Picture WEI-GUO YIN, CHIA-HUI LIN, WEI KU, Brookhaven National Laboratory — The novel block checkerboard antiferromagnetism in Fe-vacancy-ordered insulating $K_{0.8}Fe_{1.6}Se_2$ is investigated theoretically [1]. Neither of the Fermi surface nesting and the Mott insulator scenarios, which were widely employed to model previous Fe-vacancy-free iron-based superconductors, is supported by our first-principles analysis of its electronic structure including unfolded Fermi surface, band gap, and orbital polarization. Instead, the orbital-degenerate double-exchange model, previously proposed to unify the metallic collinear and bicollinear antiferromagnetism of iron-based superconductors, is found sufficient to explain this insulating spin order as well as associated quantum magnetic transition induced by tetramer lattice distortion. Our findings demonstrate that the iron-based superconductors be universally described in the framework of coexisting itinerant and localized electronic states, which are coupled by Hund's rule coupling on the Fe atoms. Work supported by DOE DE-AC02-98CH10886.

[1] W.-G. Yin, C.-H. Lin, and W. Ku, arXiv:1106.0881v1.

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