

Abstract Submitted
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Block versus Stripy Antiferromagnetism in the Fe-Based Spin-Ladder Materials (Ba,K)Fe₂Se₃¹ WEI-GUO YIN, LIMIN WANG, WEI KU, Brookhaven National Laboratory — We present a theoretical study of the novel magnetism in the insulating two-leg spin-ladder material Ba_{1-x}K_xFe₂Se₃, which exhibits a spontaneous formation of block and stripy antiferromagnetic spin orders in the Ba and K end members, respectively, and spin glass behavior in between. The bare spin susceptibility calculated with the first-principles electronic structure is found to remain qualitatively unchanged upon hole doping (substitution of K for Ba), ruling out the simple scenario of Fermi surface nesting. We show that these doping-dependent spin orders can be explained by use of a model of coexisting itinerant and localized electronic states on the Fe atoms, which are coupled by Hund's rule coupling. Our results reveal a strong spin frustration coming from the competing antiferromagnetic superexchange and ferromagnetic double-exchange interactions in this system, and unify its magnetism with that of the iron-based superconductors [1,2]. Work supported by DOE DE-AC02-98CH10886. [1] W.-G. Yin, C.-C. Lee, and W. Ku, Phys. Rev. Lett. **105**, 107004 (2010). [2] W.-G. Yin, C.-H. Lin, and W. Ku, Phys. Rev. B **86**, 081106(R) (2012).

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