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Mott transition in multi-orbital Hubbard models for iron pnictides RONG YU, QIMIAO SI, Department of Physics and Astronomy, Rice University — The bad-metal behavior of the iron pnictides has motivated a theoretical description in terms of a proximity to Mott localization. Since the parent compounds of the iron pnictides contain an even number of 3d-electrons per Fe, it is important to determine whether a Mott transition robustly exists and the nature of the possible Mott insulating phases. We address these issues in multi-orbital Hubbard models for the parent iron pnictides using a slave-spin approach. We show a metal-to-Mott-insulator transition in xz and yz orbitals generally exists in these models [1]. The nature of the metal-to-insulator transition may be strongly affected by the Hund's couplings. For certain values of Hund's couplings, we show there is a orbitally selective metal-to-insulator transition: the transition to a Mott insulator in the xz and yz orbitals takes place at the same critical coupling as the transition to either an orbitally polarized insulator or a band insulator in the other orbitals. Implications for the electronic and magnetic properties of the iron pnictides are discussed.

[1] R. Yu and Q. Si, arXiv:1006.2337.

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