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Impact of Hund's rule on the physics of the Fe-based superconductors

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The Hund's rule coupling J_H , as opposed to the Coulomb interaction (Hubbard) U, plays a dominating role in the Fe-based superconductors. The strong Hund's rule coupling combined with the multi-orbital nature and special valence of the Fe 3d shell, as well as the small crystal fields from the surroundings of an Fe atom, lead to many experimental consequences. In this talk, I will discuss the insights from first-principles calculations based on a combination of density functional theory and dynamical mean field theory. I will demonstrate the observable effects of Hundsness on transport, optical conductivity, X-ray spectroscopy, angle-resolved photoemission spectroscopy, spin/magnetic excitations, and so on.

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