Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Hund's metal physics in iron-based superconductors
GABRIEL KOTLIAR, ZHIPING YIN, KRISTJAN HAULE, Department of Physics and Astronomy, Rutgers University — The role of Hubbard U and Hund's J in a material depends on the energy scale of the crystal field splitting. In transition metal oxides, the crystal field splitting is usually considerably larger than Hund's J thus Hubbard U plays the dominating role. However, the crystal field splitting in iron-based superconductors is substantially smaller and the physics in this family is governed primarily by Hund's rule. In this talk, we will show that the combination of density functional theory and dynamic mean field theory properly incorporates the Hund's physics as well as realistic band structure thereby is well suited to capture and predict a wide range of physical properties and their trends in iron pnictides and chalcogenides, such as optical conductivity, x-ray spectroscopy, Fermi surface, magnetic ordering and moments, spin excitations, effective masses and so on. We will demonstrate two important mechanisms operating in this family, namely, Hund's blocking and Kinetic frustration. The importance of electronic correlation caused by the Hund's physics and its relation to various experimental observations will also be discussed.

Gabriel Kotliar
Department of Physics and Astronomy, Rutgers University

Date submitted: 09 Nov 2011 Electronic form version 1.4