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Ordered and Disordered Magnetic States in Mott insulators: Insights from Spectral Density Functional Theory[1] QUAN YIN, SERGEJ SAVRASOV, New Jersey Instiute of Technology, GABRIEL KOTLIAR, Rutgers University — Self-consistent many body + electronic structure calculations using dynamical mean field based spectral density functional method are presented to study various magnetic states in several Mott-Hubbard insulators such as classical transition metal oxides MnO, FeO, CoO, NiO, as well as FeS. Solution of the Anderson impurity problem in these strongly correlated systems will be approximated by using the Hubbard I method. Comparison will be made for the electronic spectral functions and magnetic moments in both ordered and local moment regimes. The results will be contrasted to less rigorous LDA+U calculations. Prospects for theoretical predictions of the Neel temperatures within this method will be discussed.

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