

## **Predictive Capabilities for Strongly Correlated Systems: Spectral Density Functional Theory and its Applications**

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Density functional theory (DFT) known to work well for weakly correlated materials fails to attack real strongly correlated phenomena, and recent progress in understanding those using many-body model-hamiltonian-based dynamical mean-field theory (DMFT) has triggered developments of new approaches for computational material science in searching for alternatives to DFT. In this talk, one of such new techniques, a spectral density functional theory [1], which considers total free energy as a functional of a local electronic Green function, will be discussed. Local dynamical mean-field theory is seen as an approximation within this functional approach, which can be used for practical calculations. Illustrations of the method to compute total energies, local excitational spectra, lattice dynamics and other properties of strongly correlated systems will be given.

[1] S. Savrasov, G. Kotliar, and E. Abrahams, *Nature* 410, 793 (2001).