MAR08-2007-005036

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

Computational Approaches for Strongly Correlated Materials: an Electronic Structure Theory Perspective.

SERGEY SAVRASOV, University of California Davis

Density functional theory 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 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, which considers total free energy as a functional of a local electronic Green function, will be discussed. Applications of the method to compute energetics, spectroscopy, lattice dynamics and exchange interactions of classes of materials such as heavy fermion and high temperature superconductors as well as actinide systems will be given.