초청강연 I-1

Electronic Structure Calculations with Dynamical Mean Field Theory

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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 [1,2], which considers total free energy as a functional of a local electronic Green function, will be discussed. Local dynamical mean-field theory, LDA+U, LDA+DMFT are seen as various approximations 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 various systems will be given.

[1] S. Savrasov, G. Kotliar, and E. Abrahams, Nature 410, 793 (2001).
[2] X. Dai, S. Y. Savrasov, G. Kotliar, A. Migliori, H. Ledbetter, E. Abrahams, Science 300, 953 (2003).