

COLLOQUIUM

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Merging Green's Function-based Many-Body and Density Functional Theory

For Materials Science

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Abstract

Ground-state density functional theory (DFT) is the most popular way to compute energies, electron densities, and nuclear frameworks in condensed matter physics, materials science, and chemistry. Its time-dependent generalization (TDDFT) is also a popular way to compute time-varying electron densities and excitation energies. Despite their computational efficiency, both ground-state and TDDFT seriously break down for band-gaps of semiconductors or insulators, strongly-correlated systems, dissociation of molecules, charge-transfer excitations, and excitonic peaks. The source of most these failures is the self-interaction error inherent in DFT.

Nonlocal many-body approximations based on the Green's function reach beyond DFT and can potentially eliminate these deficiencies. Some of these approaches can be interpreted within DFT.

One of these approximations is the particle-hole Random Phase Approximation (RPA) which is becoming a standard method beyond semilocal DFT. RPA naturally incorporates weak interactions and eliminates self-interaction error in the exchange energy. RPA is not completely perfect, however, and suffers from self-correlation error as well as an incorrect description of short-ranged correlation. To improve upon RPA, an exchange(-correlation) kernel can be included in the calculation of the correlation energy. Kernels applied to the ground-state can be naturally extended to time-dependent processes within TDDFT and can potentially be applied within the Green's function-based *GW* method for quasiparticle energies.

In this talk I will reveal the strengths and limitations of these approximations through some materials problems such as structural phase transitions and surface energies.

Monday, March 12, 2018 at 3:00 pm
SERC, Room 116
Refreshments will be served at 2:45 pm