Laboratoire des Solides Irradiés, UMR 7642

SEMINAIRE

Lundi 15 novembre 2010 à 10 h 30
Amphi Becquerel

Harnessing molecular excited states with Lanczos chains

STEFANO BARONI

Professor. of theoretical condensed-matter physics and. head of the Condensed Matter Theory & Simulation Sector, Scuola Internazionale Superiore di Studi Avanzati (SISSA Trieste)

Abstract :

Much progress has been made in recent years in the simulation of optical spectroscopies, thanks to the deployment of techniques such as time dependent DFT (TDDFT), many-body perturbation theory (MBPT), or a combination of the two. However, the numerical difficulties that affect most of the existing implementations of these techniques have limited so far their application to the lowest-lying portion of the spectrum of systems of a few to a few tens of inequivalent atoms at most: one to two orders of magnitude smaller than those currently treatable by ground-state DFT techniques.

Recent algorithmic advances, which use a generalization to finite frequency of some of the ideas embodied in density-functional perturbation theory (DFPT) and based on a Liouville-Lanczos approach to TDDFT, are allowing us to simulate the optical spectra of systems as large as a few hundreds of inequivalent atoms, thus considerably reducing the size gap between ground- and excited -state simulations.

In this talk I will retrace the path that has lead from DFPT to the Liouville-Lanczos approach to TDDFT. The crucial step of this path is the use of a Lanczos technique to avoid the calculation and use of unoccupied states of the one-electron Hamiltonian. This same idea allows one to extend the scope of GW calculations within MBPT to systems of unprecedented size, as well as to improve their accuracy. A number of applications will be presented to illustrate this path, some of the difficulties that still hinder it will be discussed, and future directions will be hinted in the light of present successes and failures.