



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
SEMINAR

Efficient Evaluation of Dielectric Response Functions: Applications to Ground State and Excited State Problems

by

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ALL INTERESTED ARE WELCOME

Abstract

Computing the dielectric response function of molecules and solids from first principles has played a significant role in the modern electronic structure theory. We have developed a technique to diagonalize iteratively dielectric matrices, in order to carry out efficient, ab-initio calculations of dispersion energies, and excited state properties of nanostructures. In this talk, I present our recent results for the binding energies of weakly-bonded molecular crystals, obtained at the EXX/RPA level of theory, and for absorption spectra of molecules and nano clusters, obtained by an iterative solution of the Bethe-Salpeter equations. We show that the ability to obtain the eigenmodes of dielectric matrices from the density functional perturbation theory, without computing single particle excited states, greatly improves the efficiency of both EXX/RPA and many-body perturbation theory calculations and opens the way to large scale computations.