Joint CQSE and CASTS Seminar

Weekly Seminar
Nov. 25, 2011 (Friday)

TIME Nov. 25, 14:30 ~ 15:30
TITLE Algorithms and Applications of TDDFT on Electronic Excited-state Properties and Dynamics
SPEAKER Prof. Wan-Zhen Liang
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Abstract

Due to the great promise between the numerical accuracy and the computational efficiency, Time-dependent density functional theory (TDDFT) has evolved into a general routine to extract the excitation energies of low-lying excited states over the last decades. To extend the TDDFT power for describing molecular photophysical and photochemical processes, one has to develop the novel algorithms to efficiently calculate TDDFT excited-state energy derivatives and numerically solve the time-dependent Kohn-Sham equations directly in real-time domain. In this talk I will report our recent works on the algorithms and applications of TDDFT on the linear and nonlinear spectroscopes, electronic dynamics and the excited-state properties of nano-size clusters.