

Joint CQSE and CASTS Seminar

Special Seminar
Apr. 25, 2019 (Thursday)

TIME Apr. 25, 2019, 14:30 ~ 15:30
TITLE A New TDDFT method for Isolated Systems
SPEAKER Prof. Xiao-Min Tong
Center for Computational Sciences,
University of Tsukuba, Japan
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Time-Dependent Density Functional Theory (TDDFT) is broadly used to study the dynamics of many-electron systems from a single atom to a crystal. In this talk, I will briefly review some existed TDDFT packages and introduce our newly developed TDDFT method for isolated systems with Fast Fourier Transform algorithm. Then, I will focus on the key components, like time-propagator, Poisson Solver and how to improve the exchange-correlation functional by considering the self-interaction-correction without increasing the numerical affords. Some examples will be presented to show the validity of the new TDDFT method.

