

# Joint CQSE and CASTS Seminar

**Weekly Seminar**  
**Dec. 16, 2011 (Friday)**

TIME Dec. 16, 14:30 ~ 15:30  
TITLE Some excited-state studies within the time-dependent density functional theory  
SPEAKER Dr. Yihan Shao  
Q-Chem, Inc.  
PLACE Rm716, CCMS & New Physics Building, NTU

## Abstract

We will discuss the time-dependent density functional theory (TDDFT) for studying molecular excited states, and focus on: a) a QM/MM excited-state study on luciferase, and b) the performance of non-collinear spin-flip TDDFT on small molecules.

