

Joint CQSE and CASTS Seminar

Weekly Seminar
Apr. 20, 2012 (Friday)

TIME Apr. 20, 14:30 ~ 15:30
TITLE Recent developments in accurate electronic structure theories
for photochemistry
SPEAKER Dr. Toru Shiozaki
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Our recent developments in multireference electron correlation theories will be presented. I will review the so-called explicitly correlated (or F12) multireference theories that provide predictive accuracy for small systems with moderate costs. I will also show the extended multi-state CASPT2 method that is useful for qualitative understanding of large systems. The prospect of combining them for large-scale photochemical applications will be discussed in the talk.

