The 889th IMS colloquium

Theoretical aspects of the molecular dynamics and spectroscopy involving in electronically excited states

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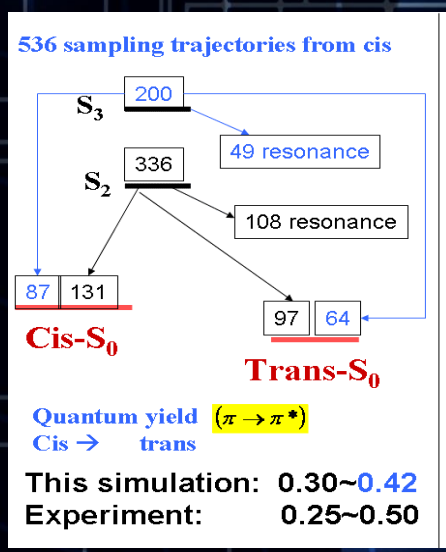
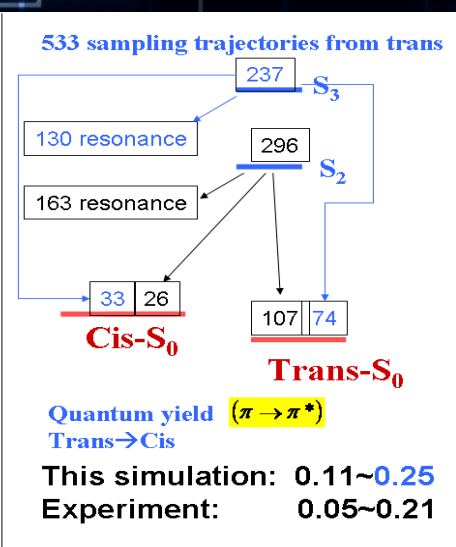
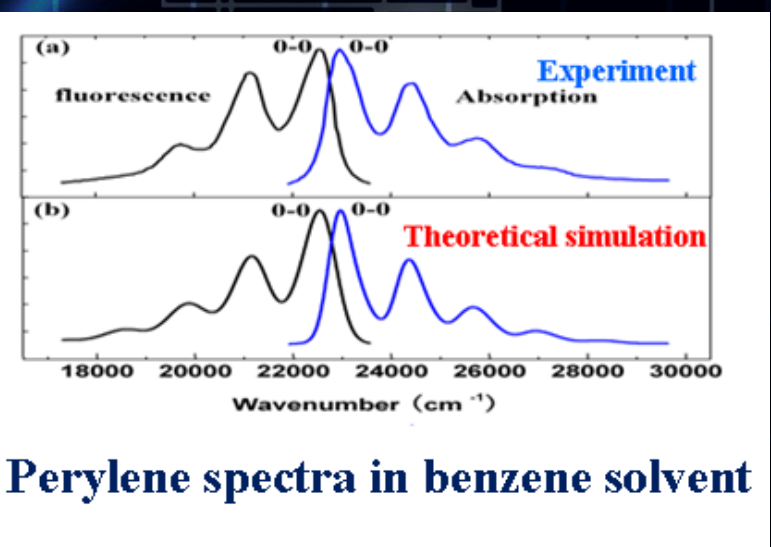
Date & Time: 2016/6/15 (Wed.) 16:00-
Place: IMS Research Building Room 201

Born-Oppenheimer approximation that separates slow nuclear motion with fast electronic motion is essential for solving Schrödinger equations and thus it introduces electronically excited states. Various ab initio quantum chemistry methods are developed to calculate excited-state potential energy surfaces and couplings among them. On the other hand, various quantum mechanical, semi-classical and classical mechanical methods or mixed of them are also developed to simulate electronically excited-state molecular dynamics and spectroscopy. In order to perform large-scale simulation, simple and accurate theoretical methods are essential. We have developed analytical switching trajectory surface hopping algorithms step-by-step to deal with conical intersections and intersystem crossings on an equal footing for nonadiabatic photophysical and photochemical processes. We have also developed analytical corrections on Franck-Condon factors with use anharmonic and damping oscillators to improve molecular spectroscopy simulation in both gas and solution phases. Various real-system applications in comparison with experimental observations are briefly addressed.







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