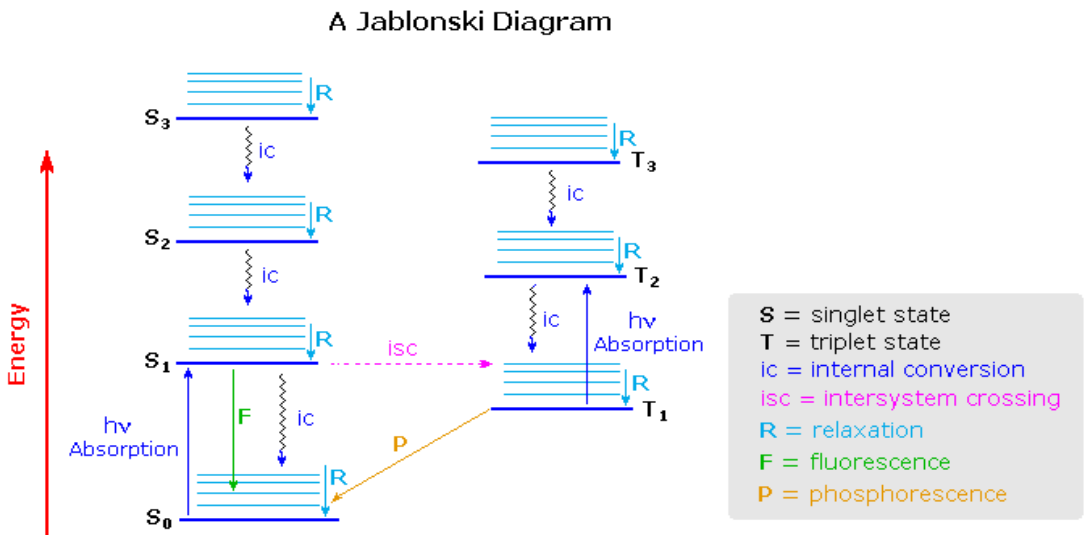
Extension: 56582 Email: cyzhu@mail.nctu.edu.tw

Prof. Chao-Yuan Zhu / Department of Applied Chemistry

Excited-State Molecular Dynamics & Spectroscopy , Computational & Theoretical Chemistry

When molecule absorbs light from electronic ground state to excited states, it undergoes nonadiabatic chemical reactions or isomerizations (Figure 1) and fluorescence according to Franck-Condon Principle (Figure 2). Actually, experimentalists summarize photochemistry processes in the following **Jablonski Diagram** which demonstrates many complicated chemical and physical processes. Quantum yield, lifetime, vibronic band structures, intensities and etc. of those processes can be measured experimentally. We want to use computational and theoretical chemistry methods to simulate those experimentally observed processes and interpret intermediate physical insights. We use computational packages (like Gaussian 09) combined with our group made computational codes (like on-the-fly trajectory surface hopping and anharmonic corrections) to perform simulations.



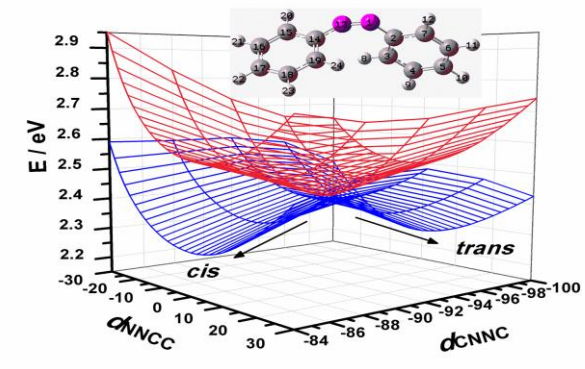


Figure 1

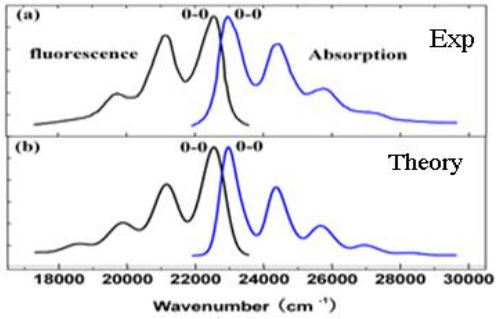


Figure 2