We have investigated wide varieties of “excited-state chemistry” and established “theoretical fine spectroscopy” with the SAC-CI method. In this talk, we present our recent challenges to photochemistry of biological chemosensor, organic light-emitting diodes, and inner-shell electronic processes.

Fluorescent artificial chemosensor has been intensively developed, since it enables the direct and real-time measurements of the enzyme activities. Recently, a novel molecular fluorescent probe which can selectively recognize the phosphoprotein has been developed. This fluorescent artificial chemosensor shows drastic fluorescence change in the presence of Zn\(^{2+}\) ion in solution. We have studied the photochemistry of this fluorescent probe and the photoinduced electron transfer mechanism.

Organic light emitting diode (OLED) is one of the promising candidates for the next generation electro-optical devices such as panel display. It is important to predict the photo-physical properties of OLED theoretically for the molecular design. We studied the absorption spectra, emission spectra, and excited-state geometry of some OLED molecules like polyphenylenevinylene, fluorene-thiophene, and Ir complexes.

Developments of high-resolution x-ray photoelectron spectroscopy and accurate theoretical methods have allowed precise knowledge and assignments of the inner-shell electronic processes. Recently, we have investigated the various kinds of core-electronic processes like core-electron binding energy, inner-shell satellite spectra with vibrational progression, and valence-Rydberg coupling and its thermal effect. We present here the summary of our recent works on core-electronic processes.


