HOKKAIDO UNIVERSITY

AMBITIOUS LEADER'S PROGRAM

Fostering Future Leaders to Open New Frontiers in Materials Science

Ambitious 物質科学セミナー

Photochemistry and Photophysics of Transition Metal Complexes: Quantum Studies

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平成 27 年 3 月 24 日(火)15:30~16:15

北海道大学 理学部 6 号館 6－204-(02)

This lecture will illustrate the progress made in the past few years in our understanding of complicated mechanism underlying photophysical and photochemical processes in transition metal complexes taking into account environment and spin-orbit effects. Three recent applications, based on state-of-the-art quantum chemical methods, will illustrate the complexity at different scales. The first part of the lecture is dedicated to the spectroscopy and photophysics of Ru (II) complexes used as DNA intercalators. The influence of the environment on the optical properties will be discussed under the light of recent results obtained by means of DFT and QM/MM calculations performed on ruthenium polypyridyl complexes. The second part of the lecture reports a comprehensive theoretical study of the ultra-fast steps leading to ligand *trans-cis* isomerization of Rhenium (I) tricarbonyl diimine complexes under visible light. The chosen molecule is representative of a wide class of compounds largely studied experimentally. The electronic absorption spectroscopy and the photophysics of [Re $(CO)_3$(2,2'-bipyridine (t-4-styrylpyridine))$^+$ and derivatives are analyzed on the basis of *ab initio* CASSCF/MS-CASPT2 and spin-orbit calculations. In a last illustration the simulation of ultra-fast intersystem crossing processes by means of TD-DFT calculations and wavepacket propagations will show how the standard image based on singlet-triplet transitions and heavy atom effects is being undermined in the case of Re (I) complexes investigated by fs laser luminescence experiments.

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