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Computational simulation of U.V. electronic absorption spectrum by time-dependent density function theory (TDDFT)

O Xiaojing Wang[1], Chen Lv[1], Akira Endo[1], Momoji Kubo[1] and Akira Miyamoto[1)2)]

[1]Graduate School of Engineering, Tohoku university

[2]NICHe, Tohoku University

Introduction

The charge transfer between metal and ligand (MLCT or LMCT) occurs easily in organometallic complexes. The properties of MLCT or LMCT excited states have been exploited recently for practical applications in areas such as solar energy conversion, chemical sensing, and photo-catalysis. Computational simulation of electronic absorption spectrum is considered as important method to supply information of charge transfer excited state. In this presentation we will do a research on the electronic absorption spectrum and charge transfer excited state by the combination methods of time-dependent density function theory and different self-consistent-field technique.

Computational methods

The simulated electronic absorption spectrum is obtained by performing with the ADF-RESPONSE module which is an extension of the Amsterdam Density Functional (ADF) program system. The excited states were calculated by differential self-consistent-field density-functional-theory (ΔSCF-DFT), in which the separate self-consistent-field calculations were performed to optimize the ground state and the appropriate excited state determinants.

Results and discuss

onic absorption spectra of the series of the complexes Cp_2MCl_2 and $Cu(phen)_2^+$ have been investigated in this work. For the series of Cp_2MCl_2, the HOMO's are primarily ligands in character, the LUMO's is mainly metallic d orbital. With the transition from ground state to excited state, the electron transferred from ligands to the central metals(LMCT). However for the series of $Cu(phen)_2^+$, the HOMO's is primarily d orbital of metal, the LUMO's is primarily ligands. The first excitation was assigned to the excitation of MLCT excitation. The excitation energies obtained by our calculation are agreement well with the experimental values.