My Internship in Toulouse

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In quantum chemistry, various symmetry-adapted (SA) and broken-symmetry (BS) computations have been performed for the strongly correlated transition metal compounds such as the perovskite-type transition metal solids and manganese oxides in Photosystem II. In our previous work, we have examined the utility and applicability of BS hybrid-density functional theory (DFT). On the other hand, SA configuration interaction (CI) is more desirable for obtaining the physical constants precisely than hybrid-DFT, though they are difficult to perform calculations for larger clusters. In order to examine the magnetic interactions of the biological transition metal complexes, it is needed to take advantages of both solutions. For example, more precise calculation is necessary for their active sites. On the other hand, as the ligand effects are crucial to decide their magnetic properties, larger clusters including ligands should be considered.

In this study, I have learned how to perform SA CI calculations such as CASSCF and difference-dedicated CI (DDCI) for the MMX chain of $Pt_2(dta)_4I$ ($dta=CH_3CS_2^-$), and have examined the ligand effect of the platinum dimer by the use of CASCF and DDCI. We have

constructed three types of cluster models such as (1) $Pt_2(CH_3CS_2^-)_4$, (2) $Pt_2(CHS_2^-)_4$ and (3) $Pt_2(CH_2S_2^-)_4$ to examine the delocalization effect of the dta ligand. While the delocalization effects by the π bonding are remained in the case of (1) and (2), the π bonding vanishes in the case of (3). It has been confirmed that the delocalization is caused by the π bonding between carbons in the dta ligand. We are going to report these result in the paper.

In this dispatch, my aim to visit Toulouse is to activate interpersonal contact between Osaka university and université Paul Sabatier. During my staying in Toulouse, I could master how to run the DDCI calculations and discuss about their results, improving my English and French. Now, I am contacting them by e-mail and continuing our collaboration.

In order to research in the foreign countries, speaking English is required as the minimum condition. Otherwise, the research is not carried out smoothly. In addition to this, learning their culture is very important so as to know them deeply. I hope that students and younger assistants in Osaka university can continuously have the chance to visit foreign

countries.

French Dinner with My Colleagues