

Report for Interdisciplinary research startup

1. Name of project leader : **Yuichi Kitagawa**

2. Project title : **理論計算を含めた発光錯体合成**

Synthesis of luminescent complexes containing theoretical calculation approach

3. Report

Lanthanide complexes show characteristic emission with high color purity and prominent chiroptical properties; thus, they have garnered considerable attention as luminescent materials. However, the lack of understanding of their detailed electronic structure has suppressed the development of design strategies for targeted photo-function of lanthanide complexes. Therefore, I have undertaken joint research with computational chemists at WPI-ICReDD and set up the workstation in our group (experimental chemists) to simulate the electronic structures of lanthanide complexes.

4. Research achievement

1. Y. Kitagawa, M. Kumagai, T. Nakanishi, K. Fushimi, Y. Hasegawa*, "The role of π -f orbital interactions in Eu(III) complexes for an effective molecular luminescent thermometer", *Inorg. Chem.* 59, 5865 (2020).

2. Y. Kitagawa, M. Kumagai, P.P. Ferreira da Rosa, K. Fushimi, Y. Hasegawa*, "First demonstration of π -f orbital interaction depending on coordination geometry in Eu(III) luminophore", *Dalton Trans.* 49, 3098 (2020).

3. Y. Kitagawa, F. Suzue, T. Nakanishi, K. Fushimi, T. Seki, H. Ito, Y. Hasegawa*, "Stacked nanocarbon photosensitizer for efficient blue light excited Eu(III) emission", *Commun. Chem.* 3, 1 (2020).