

Report for newly appointed faculty startup

1. Name of project leader : **Kosuke Higashida**
2. Project title: **Design of novel transition metal catalysts using prediction by DFT calculation**
3. Report

The reporter started the investigation of high-performance catalyst molecules for activation of the inactive bond based on the estimation by computational chemistry. DFT calculation using the AFIR method gave the key transition state structure for cleavage of inactive bonds with transition metal catalysts, and these results allowed to find the high-performance catalyst candidate, which possibly activate inert bond with low energy barrier. The above-mentioned support fund was used to purchase the laboratory table, shelves, glassware, and reagents, which are necessary for setting up the laboratory and conducting synthetic experiments. Additionally, this support helped to join conference for gaining the information about the recent development of the design of catalysts.

4. Research achievement