MERIT Long-term Overseas Dispatch Report

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Overview

I stayed in the Müllen group in Maxplank Institute in Germany from 2019/8/1 to 2019/10/29 for research. In this report, I will report the background, research and what I thought during my stay in Germany.

Background

I've been working on the development of iron-catalyzed C–H activation reaction since I joined the Nakamura group. Developing new reactions based on their mechanism is a fundamental skill that is needed for organic chemistry, which means that reaction methodology field is centered in the field of organic chemistry. However, I have come to feel after three years that the field of methodology is relatively isolated from other fields. In order to think about how this field should proceed in the future and how chemistry should proceed, I decided to stay the Müllen group, where they work on the development of new carbon materials and use organic reactions as a tool to synthesize their target compounds.

Research

Although I cannot describe the details, I mainly worked on the synthesis of new polycyclic aromatic hydrocarbons (PAHs) through transition-metal-catalyzed C–H activation and on-surface synthesis of a nano-porous graphene.

Recently PAHs have attracted much attention due to their intriguing electronic and optical properties. However their synthetic routes are discrete and when they want to have an access to a new PAH, they have to think of a new synthetic route from the beginning and synthesize through several steps. If we could achieve C–H functionalization of an existing PAH, we would have a quick access to new PAH cores. After optimization of the reaction conditions, iridium-catalyzed C–H borylation was found to be effective for the PAH and the following palladium-catalyzed cross-coupling

gave a new π-extended PAH. The properties of the product are now under investigation by collaboration with physicists.

The synthesis of the monomer for the on-surface synthesis of a nano-porous graphene was also conducted. It is known that graphene possesses 0 bandgap but it can be assumed that a periodic defect can create a bandgap on graphene. Based on this idea, I designed the monomer that is suitable for this purpose and completed the synthesis. The obtained monomer will be sent to the collaborators.

What I thought during my stay in Germany

When I was working on both projects, where the final product has to be obtained no mater what kind of reaction I use, I found that the requirement for the reaction is very high. Especially for PAHs, the activity of the catalyst has to be high enough to be active even at low concentration of the substrate because usually the solubility of PAHs is low. The use of strong oxidant or reductant has to be avoided to prevent direct oxidation or reduction of the PAH substrate.

In general, it was a very nice experience to come up with a new project by myself and design and synthesize the molecule in a period of three months.

Acknowledgement

I would like to thank Prof. Klaus Müllen and Project Leader Akimitsu Narita for fruitful discussions, Prof. Eiichi Nakamura for giving me this great opportunity, and GRASP for their big support including financial support.