Usage Report for Fiscal Year 2024

Project Title:

Rare-Earth Metal Catalysis for Multi-functional Polymer Synthesis

Name:

○ **Mengqing CHEN, Zhaomin Hou**

Laboratory at RIKEN:

Center for Sustainable Resource Science Advanced Catalysis Research Group
Advanced Catalysis Research Group

1. Background and purpose of the project, relationship of the project with other projects

Self-healing (SH) polymers are auspicious materials for diverse applications due to their ability to autonomously repair damage, thereby enhancing the durability of structural components and the reliability of electronic devices. Previous research in our group has reported SH phenomena driven by phase separation. The seminal discovery of SH-polymers consist of several types, one of which, we designate as **E/EA**, where an allylanisol (**A**) and ethylene (**E**) selectively form first an **EA**-unit, which copolymerizes with **E**. The **EA** part acts as the elastic part of the polymer, while the polyethylene part forms crystalline nanodomains that crack upon mechanical stress and crystallize again when the stress is removed. Mechanistically, the methoxy group on **A** Plays a key role controlling the coordination chemistry around the rare-earth metal employed as a catalyst in the polymerizations (i.e., heteroatom-assisted olefin polymerization, HOP) hence enabling the selective formation of the **EA** unit. This study aims to expand SH polymer applications through molecular design and mechanistic study. We incorporated ferrocene, valued for its stability, reversible redox behavior (Fe^{2+}/Fe^{3+}), and electron-donating properties, which enhance electron mobility in molecular wires and nanoelectronics.

2. Specific usage status of the system and calculation method

None.

3. Result

None.

4. Conclusion

None.

5. Schedule and prospect for the future

None.

6. If no job was executed, specify the reason.

At the time of reporting, the project had not progressed to the stage where calculations were required.