Usage Report for Fiscal Year 2022

Project Title:

Computationally assisted polymer synthesis

Name:
○Hao WANG
Laboratory at RIKEN:
Organometallic Chemistry Laboratory

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

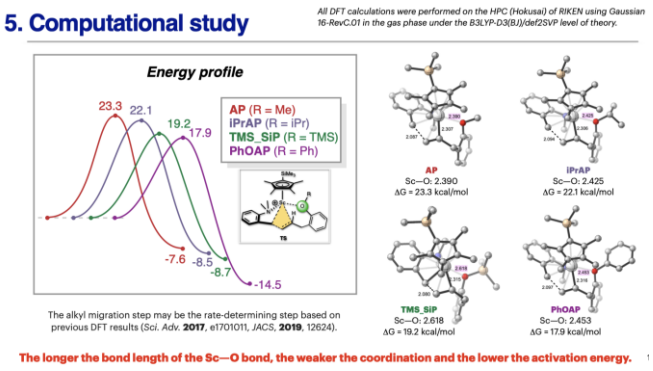
The essence of chemical reaction is to study the interaction between electrons. The microscopic electron configuration needs to be simulated by supercomputers. With the aid of supercomputers, it plays a very important role in studying current chemical reactions, especially the simulation of polymers. This method can understand not only the microscopic composition, but also can be used for the understanding of polymers and some dynamic properties, which is of great significance for the development and application of polymers. Recently, Hou and coworkers reported the synthesis of a new class of self-healing materials, formed by the copolymerization of ethylene and anisyl-substituted propylenes using a sterically demanding half sandwich scandium catalyst. I became interested in the influence of substituent on the oxygen atom of O-substituted-2-allylphenoxy ether. To clarify the influence of the substituents in the polymerization, the alkyl migration step was examined by DFT calculation.

2. Specific usage status of the system and calculation method

Gaussian 16 was used for the chemical structure optimization and transition state searching, to study the mechanism of the polymerization reaction.

3. Result

I systematically studied the alkyl migration step of scandium-alkyl bond into O-substituted-2-allylphenoxy ether bearing methyl, isopropyl, phenyl, and -TMS. Density functional theory study showed the significant influence of the substituents on the oxygen atom. This energy difference may give structural difference of the microstructure of the corresponding copolymer of ethylene and O-substituted-2-allylphenoxy ether.



4. Conclusion

With the assistance of the HPC, significant influence of the substituents on the oxygen atom of 2-allylphenoxy ether has been observed in the alkyl migration step.

5. Schedule and prospect for the future

I have resigned from RIKEN, so my account should be cancelled.

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

N.A