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Origins of selectivity and activity of olefin polymerization catalyzed by rare earth metal complexes

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Rare-earth metal complexes as a kind of polymerization catalyst usually show unique polymerization activity and selectivity and therefore afford various microstructures of the resulting polymers, not achievable via. transition metal analogues. Mechanism-based rational design of catalyst provides an attractive way towards new polymer materials with desired properties. In this context, theoretical calculations can help in many ways. Charactering catalytic active species, clarifying the mechanism behind experimental phenomenon, and dynamic modeling of polymerization process are just a few examples. With an increase in computer technology and more robust algorithms, computational chemistry has become a viable option for molecular studies in the field of polymer chemistry. In this talk, computational investigations on the molecular mechanism of polymerization catalyzed by rare-earth metal complexes will be introduced. The polymerization mechanisms of conjugated dienes, styrene, and 1-hexene will be covered in the presentation. Especially, the origins of experimentally observed regio- and stereo-selectivity as well as activity suggested by theoretical calculations will be discussed. The polymerization mechanism of lactone and vinyl polar monomers will be also included

Biography

Yi Luo received his PhD degree in Material Chemistry from Tohoku University in 2004, supervised by Prof. Akira Miyamoto. He has his expertise in computational organometallic chemistry. In the field of computational chemistry, his research interests include rare-earth metal catalyzed polymerizations. He has also contributed good works on intermetallic cooperation towards activation of chemical bond, including C=C double bond. He is active in his scientific research and often collaborates with experimentalists to discover new chemistry together. The effect of THF molecule on olefin polymerization catalyzed by rare earth metal complexes, which was a long-term concern in this field, have been clarified in his multiple research works. It has been proposed that, at the molecular level, the generation of catalytically active species and its chemical hardness could account for the polymerization activity.

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