令和 2 年度　京都大学化学研究所 スーパーコンピュータシステム 利用報告書

Simulation of radical addition and ring-opening reaction upon the radical polymerization

京都大学 化学研究所 材料機能化学研究 高分子制御合成　　Yangtian Lu

研究成果概要

This year, our lab carried out DFT calculation to simulate the reactions occurred during our designed polymerization. There were mainly three projects were highly relied on DFT calculation. The first one is to calculated the substituent effect on the copolymerization of vinyl tellurides, which were designed as the monomer for the formation of branched structure on copolymer. We systematically calculated all of the possible reaction routes during the copolymerization for all of the target substituents. The resulting calculation data will be applied for training the prediction model. The second one is to calculate the substituent and ring-size effect on the ring-opening polymerization of cyclic monomers. Through DFT calculation, we successfully proved that ring-size are the most crucial factors for the ring-opening efficiency for our designed cyclic monomer. Now we are trying to synthesize the cyclic monomer according to the calculation results. The third one is to calculated substituent effect on the oxidation reaction of designed polymer backbone, which potentially perform as polymer degradation reaction. Currently, we are still trying to screening the potential substituent.