Metallocene Catalysts on Carbon-based Nano-materials

Baekhap Choi¹, Juno Lee¹, Seungjun Lee², Jae-Hyeon Ko³, Kyoung-Seok Lee⁴, Junghoon Oh², Yong-Hyun Kim³, Insung S. Choi¹, Sungjin Park²*

¹Department of Chemistry, KAIST, ²Department of Chemistry, Inha University, ³Graduate School of Nanoscience and Technology (WCU), KAIST, ⁴Center for analytical chemistry, Korea Research Institute of Standards and Science

Transition metal-based organometallic complexes have shown great talents as a catalyst in various reactions. Designing organic molecules and coordinating them to such active centers have been a promising route to control the catalytic natures. Metallocene, which has transition metal atoms sandwiched by aromatic rings, is one of the representative systems for organometallic catalysts. Group 4-based metallocene catalysts have been most commonly used for the production of polyolefins, which have great world-wide markets in the real life. Graphenes and carbon nanotubes (CNTs) were composed of extended sp² carbon networks, showing high electron mobility as well as have extremely large steric bulkiness relative to metal centers. We were inspired by these characteristics of such carbon-based nano-materials and assumed that they could intimately interact with active centers of metallocene catalysts. We examined this hypothesis and, recently, reported that CNTs dramatically changed catalytic natures of group 4-based catalysts when they formed hybrid systems with such catalysts. In conclusion, we produced hybrid materials composed of group-4 based metallocenes, Cp₂ZrCl₂ and Cp₂TiCl₂, and carbon-based nano-materials such as RGO and MWCNT. Such hybrids were generated via simple adsorption between Cp rings of metallocenes and graphitic surfaces of graphene/CNT. The hybrids showed interesting catalytic behaviors for ethylene polymerizations. Resulting PEs had significantly increased Mw relative to those produced from free metallocene-based catalytic systems, which are not adsorbed on carbon-based nano-materials. UHMWPEs with extremely high Mw were obtained at low Tp.

Keywords: Metallocene catalysts, Graphene, CNT, Nano-materials, UHMWPE