Design of Lanthanidocene Catalysts for Syndioselective Styrene–Ethylene Homo and Copolymerization: a Joint Experimental and Computational Effort

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Syndiotactic polystyrene (sPS) is an attractive engineering plastic but its high melting point and brittleness are two main drawbacks that limit its processability. Stereoselective copolymerization of styrene with other monomers such as ethylene is an interesting approach to tackle these issues. However, the copolymerization of those two monomers is quite challenging due to their strikingly different reactivity. Only group 3 catalysts, such as those independently disclosed by some of us and by Hou and co-workers, are really effective for this purpose, enabling incorporation of small amounts of ethylene and a high stereocontrol.

In this lecture we will discuss experimental and DFT computational studies performed on a series of neutral ansa-lanthanidocene and cationic hemi-lanthanidocene catalysts for the production of sPS and sPS-PE. We will highlight the main factors that control the effectiveness of syndioselective styrene homopolymerization and styrene–ethylene copolymerization.