Mechanistic trends from computational chemistry for the design of redox switchable catalysts

Thibault Cantat

INOR: Division of Inorganic Chemistry

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Thibault Cantat, thibault.cantat@cea.fr

DRF / IRAMIS / NIMBE / LCMCE, CEA, Gif Sur Yvette, France

Abstract:The search for efficient switchable catalysts is a challenging yet appealing task in polymer science as it could pave the road to tailor-made block co-polymers. In this context, an elegant strategy relies on exploiting the reactivity of metal complexes featuring a redox-active center (located either on the supporting ligand or the metal itself) to differentiate between two monomers.
In this contribution will be presented and discussed computational mechanistic results, carried out in close collaboration with the Diaconescu group at UCLA, on the use of redox switchable catalysts for the ring opening polymerization of cyclic esters with lanthanide-based catalysts.