Computational methods and approaches for olefin metathesis and homogeneous catalysis

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We use a combination of computational methods, ranging from tight binding approached and density functional theory to domain-based local pair natural orbital coupled-cluster method and symemtry-adopted perturbation theory to accurately describe the olefin metathesis reaction catalyzed by ruthenium-based complexes. We show that in many cases we can obtain accuracy in the 1-2 kcal/mol range, exploring in details the different mechanisms of initiation and decomposition of ruthenium-based catalysts and providing key structure-activity relationships, with the aim to facilitate the design of new, more efficient catalyst tuned to specific substrates and reaction conditions [1]. We also used similar approached to study the decomposition of ruthenium metathesis catalysts. We further extend our studies to designing new ligands for novel transition metal complexes and design new catalysts for important chemical reactions [2]. In particular we show that the newly designed amino imidazoline-2-imine ligand that can stabilize the B=O double bond as well as a series of five-membered cyclic triel(I) carbenoides.

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