

A computational perspective of olefins metathesis catalyzed by N-heterocyclic carbene ruthenium (pre)catalysts

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In recent years olefin metathesis catalyzed by N-heterocyclic carbene ruthenium complexes has attracted remarkable attention as a versatile tool to form new C=C bonds. The last developed (pre)catalysts show excellent performances, and this achievement has been possible because of continuous experimental and computational efforts to understand the laws controlling the behavior of these systems. This perspective talk rapidly traces the ideas and discoveries that computational chemistry contributed to the development of these catalysts, with particular emphasis on catalysts presenting a N-heterocyclic carbene ligand.