

Computational Studies of Reaction Mechanisms in Homogeneous Catalysis

Eric Clot

For multiple institutions use a b (centered, arial, 11)

Institut Charles Gerhardt
Université de Montpellier, CNRS
Place Eugène Bataillon
34095 Montpellier Cedex
eric.clot@umontpellier.fr

The presentation will highlight various aspects of transition metal catalyzed transformations that can be addressed by computational studies: activity, selectivity, kinetic aspects, ligand electronic properties. The purpose is to show, through various examples, the breadth of information that can be provided by computational studies, and how the latter are a necessary complementary tool to many experimental studies.