SOCIÉTÉ CHIMIQUE DE GENÈVE

Du modèle vers le système réel : un dialogue expérience/théorie en chimie organométallique

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Computational studies of transition metal complexes can now give very useful informations to the experimental chemist provided that a robust accurate method is used and that realistic models of the experimental systems are considered. The density functional method is unanimously recognized as a method of choice.

We have used the DFT method and the hybrid QM/MM method for the largest systems. We will show how the combination of simple models and more elaborate models can be used for analyzing the experimental results. We will illustrate our points from some examples which will highlight the absolute need to include the proper chemical ingredients in the calculations: ligands with proper electronic properties, ligands with proper steric properties, ligands with proper attractive weak-interactions, counter ions. We will focus mostly on processes that involve the interaction of a metal center with the CH bond of a ligand or molecule and the associated C-H activation process in some cases.

Conférence présentée le : LUNDI 2 MAI 2005 À 17H30

Université de Genève - Bâtiment Sciences II

Auditoire P.-F. Tingry (A 150)

30, quai Ernest–Ansermet, Genève

LA CONFÉRENCE EST PUBLIQUE