

Computational chemistry applied to the understanding of the catalytic activity of silica supported transition metal complexes

Xavier Solans-Monfort

Departament de Química, Universitat Autònoma de Barcelona, 08191 – Bellaterra, Spain

Chemical industry is mainly based on heterogeneous catalytic processes. However, the usual level of understanding of heterogeneous catalysis is limited, especially when compared to that of molecular catalysis. Two of the main reasons that limit the characterization of these systems are: a) the absence of a unique active site with a well-defined activity and b) The low density of active sites which makes difficult their characterization. Heterogenization of single site transition metal complexes allows obtaining a well-defined active species leading to the selectivity achieved with molecular complexes without losing the advantages of heterogeneous catalysis. Moreover, these complexes can also be used to obtain information on the reaction mechanisms of analogous heterogeneous processes. However, they still present the drawback of the low density of active sites, which limits the characterization of the supported species. In this context, computational chemistry is a complementary tool to understand the catalyst structure, reactivity and selectivity in these kind of systems.

In this communication, it will be discussed how computational chemistry can be used for better understanding the structure and reactivity of single site heterogenized metal complexes. Special attention will be focused on the design of the computational model, comparison with experiments and how the information achieved with computational tools can pave the path of further developments.