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Laboratoire de Chimie – UMR CNRS 5182

PhD Position

Monitoring active sites of metathesis catalysts: a combined operando spectroscopy and computational approach

Context

The MASCAT project is in line with a long-standing collaboration between the group of Pr. Ch. Copéret, Zurich, Switzerland and the one of Ph. Sautet, Lyon, France. It is sustained by the ANR and the SNF agencies with a join financial support. A position for PhD student is opened in modeling in Lyon starting September 2015.

Project

Industrial heterogeneous alkene metathesis catalysts are based on supported Mo and W oxides and contain very low concentrations of active sites (typically below ~1%). These sites are presumably formed under operating conditions. To improve those catalysts, a better knowledge of the active species and catalytic steps is required. We suggest an original approach based on the in situ characterization of the surface (active) sites at the molecular level at the precursor stage and during the catalytic event (in situ/operando), using in particular X-ray absorption fine structure (XAFS) and Raman spectroscopies combined with first principle density functional theory (DFT) calculations. This research project will in fine provide a detailed molecular understanding of the chemistry of metathesis catalysts and pave the way to develop industrial catalysts in a more rational way using the acquired knowledge through structure/property relationships.

The PhD in Lyon will be devoted to the theory modeling part and focus his/her research on two main tasks. To start, he/she will build a library of spectroscopic signatures (NMR, IR, …) based on DFT structural models of all surface species that are essential for the interpretation of the experimental results. Then, he/she will determine the reaction pathways for the formation of the active species and for the methatesis reaction on this active site to provide structure/activity relationship.

Applicant

The successful applicant is expected to have strong background in physical chemistry and strong interest in the application of computational modeling techniques to study chemical reactivity and spectroscopies. A Master degree is required. The student will be supported for 3 years to work towards a Ph.D. degree in Chemistry within the graduate program of the Universite de Lyon (www.edchimie-lyon.fr/). He/she will also benefit of the Ecole Normale Supérieure de Lyon environment (www.ens-lyon.eu).

Contact

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