PhD position at IFP Energies nouvelles (IFPEN)
in *Chemical Sciences*

Molecular modeling of the genesis of the active phase of a supported catalyst

Transition metal sulfides and molybdenum disulfide (MoS_2) more particularly have prompted a renewed interest thanks to their ever wider domain of applications as materials for energy. Indeed, these versatile active phases are susceptible to promote numerous reactions with high industrial and environmental concerns: hydrotreatment for clean fuels, biomass conversion, electro-/photocatalytic reactions… Hence, the understanding and the control of the elementary steps of the genesis of these catalysts from their precursors (mainly as metal oxide) remains a key challenge impacting their resulting properties.
This thesis proposes a molecular modeling approach (at the quantum level) never explored so far in order to identify the reaction mechanisms governing at the atomic scale the transformation of the oxide precursors into the catalytic MoS_2 phase dispersed on a alumina support. The project aims first at simulating the elementary steps involved in the sulfidation and reduction reactions of the precursors in order to identify the key descriptors (intermediates, transition states, anchoring sites…) of the activation steps of the supported MoS_2 phase. The second objective is to establish a micro-kinetic model of the activation based on the sulfidation and reduction rates calculated at the quantum level in order to provide rational guides for better controlling experimentally the activation step. In addition, the simulation of the spectroscopic features of the various key intermediates will enable a direct comparison with experimental analysis (XPS, XAS, RAMAN) available in the literature or obtained in the IFPEN laboratories.
The results will be published in international scientific journals and presented in conferences through oral communications.
This thesis is open to any student strongly motivated by research in catalysis and more particularly by learning computational chemistry methods applied to catalysis, in close link with experiments.

Keywords: Computational chemistry, catalysis, MoS_2

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Doctoral School	ED 206, Ecole Doctorale de Chimie de Lyon, www.edchimie-lyon.fr
Co-supervisor	Dr. STEINMAN Stephan, Laboratoire de Chimie, ENS Lyon
PhD location	IFP Energies nouvelles (2/3) and ENS Lyon (1/3)
Duration and start date	3 years, starting preferably on October 1, 2018
Academic requirements	University Master degree in chemistry, catalysis, theoretical chemistry, material sciences, physical-chemistry,
Language requirements	Fluency in French and/or English, willingness to learn French
Other requirements	Ready to work with simulation tools

For more information or to submit an application, see theses.ifpen.fr or contact the IFPEN supervisor.

About IFP Energies nouvelles
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IFPEN offers a stimulating research environment, with access to first in class laboratory infrastructures and computing facilities. IFPEN offers competitive salary and benefits packages. All PhD students have access to dedicated seminars and training sessions.