PhD position at ENS Lyon
in collaboration with IFP Energies nouvelles (IFPEN)
Chemical sciences

In silico exploration of MoS_2 nano-layers for the photocatalytic reduction of CO_2

Due to the obvious global warming of the climate, it becomes urgent to find alternative pathways to produce fuels or chemicals with minimal emission of greenhouse gases. Thus, making fuels or chemicals from the solar energy is one of the most challenging routes towards this golden target. Within this framework, a promising reaction is the CO_2 reduction into alternative fuels or valuable chemicals by means of a photocatalytic process. However, considering the current state of the art, this dream is still far from reality and there is a great need of rational and theoretical approaches to identify efficient photocatalytic materials meeting the expected optoelectronic properties to harvest light photons and exhibiting simultaneously active sites to convert CO_2.
The aim of this PhD project is to explore, by state-of-the-art quantum modelling, the ability of 2H-MoS_2 as semiconductors for photocatalytic CO_2 reduction. Based on a well-defined methodology [1], this work will focus on the calculation of relevant optoelectronic descriptors (bandgap, exciton binding energy, dielectric constant, band positions…) in MoS_2 nano-layers with tunable size, 2D-morphology and doping elements.[2] The modulation of charge separation will be addressed by including the role of a relevant support in close contact with MoS2 nano-layers. Finally, the project will simulate the reaction mechanisms of CO_2 reduction including charge effect induced by the photoactivation process.

[1] BaQuais, A. et al. Chem. Mater. 2017, 29, 8679-8689.
[2] Saab, M. and Raybaud P. J. Phys. Chem. C 2016, 120, 10691-10697.

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Keywords: Computational chemistry, quantum simulation, photocatalysis, mechanisms, CO_2, MoS_2

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PhD location	Laboratoire de Chimie, ENS Lyon - France
Duration and start date	3 years, starting preferably on October 1, 2019
Employer	ENS Lyon - France
Academic requirements	University Master degree in chemistry, catalysis, theoretical chemistry, material sciences, physical-chemistry
Language requirements	Fluency in French or English, willingness to learn French
Other requirements	Ready to work with simulation tools (high performance computer, molecular modelling interface, Linux)