Laboratoire de Chimie – UMR CNRS 5182

Post-Doc position

Modelling the photo-catalytic activity of core-shell catalysts

Duration: 18months

Advisors:

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PROJET FINANCÉ PAR L'ANR – ANR – PROJECT FUNDED BY THE ANR

Context: We will study a new concept in heterogeneous catalysis based on "core-shell" structures, where the active phase (metallic nanoparticles) is covered by an oxide that is used as a support. This system contrasts from most of the reported studies. Our preliminary results highlight that TiO_2@Au@SiO_2 core-shell catalysts surprisingly show superior performances in photocatalytic hydrogen generation (10-fold higher activity) and selective oxidation of furfural (3 times better). The objective of INGENCat is to provide fundamental understanding of such core-shell catalysts and identify the corresponding active sites. Our ambition is to solve the mystery around the superior activity of these catalysts as compared to the supported materials. We intend also to shed the light around their versatile properties in heterogeneous and photocatalysis processes in the liquid phase selective oxidation of furfural.

Project: To identify the active sites of the TiO_2@Au@SiO_2 catalysts, we will build several models and determine their predicted activity using periodic DFT calculations. We will determine the influence of the catalyst structuration on the charge carriers' dynamics at the interface Au/semiconductor using mesoscale simulations with a finite element approach (COMSOL).

Appliquant: Required qualifications include a solid background in physical chemistry, catalysis and theoretical chemistry and previous experience in computational chemistry and modern languages (bash scripting, python). Very good communication skills in English are required, French language skills are beneficial.

Location: The research axis Theoretical Chemistry and Molecular Thermodynamics of the Laboratoire de Chimie is internationally recognized in the modeling of heterogeneous catalysis for more than 30 years including photoelectrocatalysis [1,2]. Situated on the ENS de Lyon campus, it beneficiates from a rich international context in a town with more that 155 000 students, renowned for its gastronomy and its cultural heritage.

Application: We look forward to receiving your email application including a letter of motivation (one page), a CV, and contact details of two referees. The email should be addressed to carine.michel@ens-lyon.fr and tangui.le_bahers@ens-lyon.fr using "INGENCAT Postdoc position" as a title.

References:

[1] M. Shahrokhi, P. Raybaud, T. Le Bahers, *ACS Appl. Mater. Inter.* **2021**, *13*, 36465
[2] S. Steinmann, C. Michel, *ACS Catal.* **2022**, *12*, 6294