Offre de thèse financée – Financed PhD thesis

Time-resolved *operando* transmission electron microscopy for heterogeneous catalysis (Paris, France)

The **Laboratoire Matériaux et Phénomènes Quantiques** of Paris Diderot University invites applications for a **3-yr PhD student position** in *operando* transmission electron microscopy for heterogeneous catalysis. The position starts in September 2018 and ends in July 2021 and is proposed in the context of an ANR project (French Agency for Research).

Thesis description: Heterogeneous catalysis is a key player in many large-scale industrial processes and holds much promise for meeting current challenges in food, water and energy supplies. In heterogeneous catalysis by metals, the potential of bimetallic nanoparticles (BiM NPs) is undeniable [1]. Indeed, alloying of metal atoms within NPs can lead to improved catalytic activity, selectivity or resistance to poisoning as compared to monometallic NPs. Presently, the capability to design novel and more efficient BiM catalysts is hampered by the lack of a detailed understanding of the mechanisms of catalytic reactions, especially because particle structure and surface composition under reaction are unknown most often.

The purpose of this thesis is to gain fundamental atomic-scale insights into the interplay between the surface structuration and catalytic properties of heterogeneous bimetallic catalysts in conditions as close as possible to catalytic test ones, i.e., pressure and temperature. The structural and catalytic properties of BiM catalysts "in action" will be characterized *operando* using time-resolved aberration-corrected transmission electron microscopy imaging and spectroscopic techniques [2] coupled to mass spectrometry (MS).

In a first step, the PhD student will focus on finalizing the development of time-resolved *operando* transmission electron microscopy (TEM). In a second step, we propose to study in *operando* conditions the structure of model and active Au-Cu BiM NPs supported on titanium oxide (TiO_2) and to address their catalytic performance in two reactions of environmental and industrial interests: the oxidation of carbon monoxide (CO) at room temperature and the selective hydrogenation of butadiene into butenes in temperature, and at ambient pressure. To guide *operando* conditions, the PhD student will also be involved in laboratory catalytic testing of Au-Cu BiM NPs using a fixed-bed reactor under gas flow [3] under the supervision of C. Louis and L. Delannoy at the Laboratoire de Réactivité des Surfaces (Pierre et Marie Curie University, Paris). He/she will also work in close collaboration with theoretical scientists involved in the ANR project to confront theory and experiments.

References

[1] O.G. Ellert *et al.*, *Bimetallic nanoalloys in heterogeneous catalysis of industrially important reactions: synergetic effects and structural organization of the active components*, Russian Chemical Reviews, 83(8) 2014
[2] C. Ricolleau *et al.*, *Performances of an 80-200 kV microscope employing a cold-FEG and an aberration-corrected objective lens*, Microscopy, 62(2) 2013
[3] L. Delannoy *et al.*, *Selective hydrogenation of butadiene over TiO2 supported copper, gold and gold-copper catalysts prepared by deposition-precipitation,* Physical Chemistry Chemical Physics, 16(48) 2014

Net salary: ~ 1400 €/monthly

Thesis requirements and qualification

The desired profile is the following: Good knowledge of materials science or solid-state physics (knowledge in electron optics and heterogeneous catalysis will be a major asset). Strong motivation to perform in a multidisciplinary environment at the frontier of physics and chemistry. Autonomy, ability to work in a team, synthetic/redaction ability and good knowledge of French and English language are requested.

Application should include:

– Cover letter in French/English motivating the candidate interest in the position.
– Names and contact information of at least one reference.
– Up-to-date CV with education history and research experience.
– Copy of university marks at the bachelor and Master levels.

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