



PhD project (funded)

Design of advanced carbide nanocatalysts for substitution of noble metals in heterogeneous catalysis.

Context

Highly selective catalytic materials are essential in order to increase the atom economy and to reduce the carbon footprint of industrial processes for a greener chemistry. In addition, the substitution of critical metals (namely noble metals) is a key scientific, environmental and geopolitical issue for the implementation of such greener processes. Pd-based catalysts, for example, are the most efficient systems for industrial semi-hydrogenation reactions. However, Pd is a noble metal with limited resources (0.015 ppm in the earth crust) and its production is concentrated in a small number of countries (Russia and South Africa), giving rise to fluctuating prices and geopolitical concerns (Pd is on the list of the critical raw material of the EU). Transition metal carbide or nitride (TMC or TMN) catalysts (i.e. MoC, WC, MoN...) are attractive alternatives due to their metallic functionality from readily available (base) metals. The main objective of the project is to design innovative carbide and nitride nanocatalysts with optimized properties for heterogeneous catalysis. The synthesis route will involve simple, non-toxic, procedures in order to develop environmentally-friendly, cost-effective and earth-abundant alternatives to critical metals. Extensive characterizations as well as reactivity tests will be carried out in order to derive structure/activity relationships.

Work program

Catalyst design and characterization. Synthesis of new carbide/nitride catalysts in order to tune the hydrogenation selectivity. Classic and robust temperature-programmed methods will be used along with more original and challenging routes through sol-gel like methods. Various advanced characterization techniques will be used all along the synthesis (XRD, TEM, XPS...) with a significant part of synchrotron-based characterization methods (XAS).
Catalytic reactions. The TMC/TMN materials prepared will be tested in various reactions including the selective hydrogenation of acetylene or butadiene in an excess of alkenes mimicking the front-end process of purification of alkene streams (ethylene or butene).

This project is included in a larger project funded by the French National Research Agency (ANR) in collaboration with groups in Lyon (IRCELYon) and Grenoble (Institut Néel).

Qualifications

We are looking for a motivated PhD candidate with a background in materials chemistry, spectroscopy and surface chemistry. Knowledge in heterogeneous catalysis would be an asset but is not mandatory.

Starting date : October 2023.

Contact : Xavier Carrier, Prof., xavier.carrier@sorbonne-universite.fr, 33 (0)1 44 27 36 25

Laboratoire de Réactivité de Surface, Sorbonne Université, Paris. <http://www.labos.upmc.fr/lrs/>