

PhD position

Surface reactivity of intermetallic compounds catalysts

Employer: Université Paris-Sud

Workplace: Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), Orsay, France

Skill area: Materials Chemistry

Duration of contract: 3 years (starting October 2012)

Salary range: 20-25 k€/year (gross salary)

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ICMMO

The Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO) is one of the largest structures of academic research in chemistry in France. It includes about 170 permanent staff and 110 graduate students or postdoctoral fellows. It is associated with the CNRS as a joint CNRS/Université Paris-Sud laboratory and is located at the Université Paris-Sud campus in Orsay. The Institute is composed of nine scientific teams, working in the fields of chemistry for health, energy, information or environment.

PROJECT DESCRIPTION

As heterogeneous catalysis is applied in about 80% of industrial processes, the development of new highly active and selective catalysts is a great challenge. Intermetallic compounds have a huge potential as catalysts, due to the variety of their electronic and crystallographic structures which allow easy tuning their catalytic properties. Within this project, two economically important chemical reactions will be investigated: the selective semi-hydrogenation of acetylene over several Al-Co compounds, and the production of clean hydrogen by methanol steam reforming using PdIn. The rational development of these intermetallics as catalysts requires a detailed understanding of the elementary mechanisms of the reactions involved.

The interaction of relevant molecules with the surface of the selected intermetallic compounds will thus be investigated at the atomic scale using surface analysis techniques. In particular, X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and temperature programmed desorption (TPD) will be combined to follow adsorption and/or co-adsorption under various pressure and temperature ranges in order to determine the adsorption strengths of the molecules and the reaction mechanisms involved. The use of several compounds of the same binary system exhibiting well-defined electronic and crystallographic structures will allow disentangling the geometric and electronic effects on their selectivity and catalytic activity. Finally special attention will be given to the *in situ* stability of these intermetallic compounds, since it represents a crucial point to enable correlations between the observed catalytic properties and the structural and electronic properties of the compounds.

This study will be developed in the framework of a European COST action as well as a three-year project funded by the French National Research Agency (ANR) and the Deutsche Forschungsgemeinschaft (DFG), which also involves the Institut Jean Lamour (Nancy), the Max Planck Institute for Chemical Physics of Solids (Dresden) and the Crystallography Section of the Ludwig-Maximilians-University (Munich). Regular visits to these partners for meetings and joint experiments at synchrotron radiation sources are planned.

A solid background in materials science and chemistry is required. Knowledge on surface analysis will be appreciated. Motivated candidates with good academic scores should contact us as soon as possible, sending a detailed CV, two recommendation and one motivation letters. The official selection process will start by March 2012 and the candidate will be selected by June 2012. The position will be opened by October 2012.