# Extensive searches for complex intermetallic catalysts

**Title : Extensive searches for complex intermetallic catalysts**

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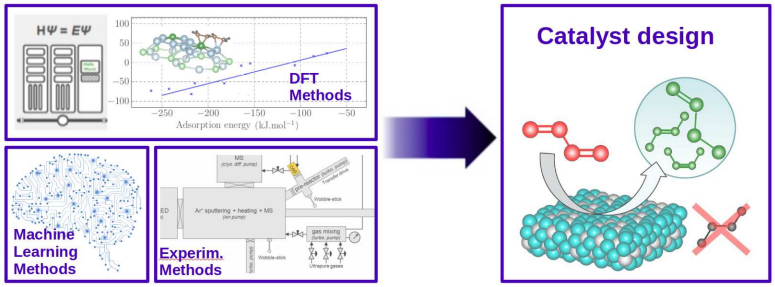
**Keywords :** Catalysis, Complex Intermetallic Compounds, Machine learning, Deep learning, Density Functional Theory




**Candidate Profile:** Strong background in physics or chemistry or materials science or machine learning with an interest for atomistic simulations. Good knowledge of quantum mechanics, as well as experience with Linux environment and python programming is required. Please send a motivation letter, CV and transcripts, along with names and contact information of two referees.

**Context and objectives :**

The objective of the thesis is to establish a deeper understanding of the relations between complex intermetallics properties and activity, selectivity and stability – the important figures of merit in catalysis. Complex intermetallic compounds belong to a class of materials characterized by a large unit cell, containing several tens to several thousands of atoms, usually arranged into regularly packed clusters of high symmetry. They offer several advantages compared to substitutional alloys, such as stability and unique combinations of electronic and crystal structure, which allows a large flexibility for tuning their properties [1,2]. Each of the thousands of binary intermetallic compounds known so far has the potential to behave as a new material, opening a vast field to be explored.

**Methods :**

Heterogeneous catalysis on complex intermetallic compounds is a quickly growing field. However, modeling the many diverse active sites and reaction paths on these complex surfaces is an open challenge. Machine learning methods coupled with Density Functional Theory (DFT) will be used to address the complex potential energy landscape of complex intermetallics catalysts. More precisely, we intend to investigate regression models such as kernel logistic regression, support vector regression, or artificial neural networks to accurately interpolate energy surfaces from a few DFT estimates [3]. The computational cost of training such models is a fraction of the costs of DFT calculations, allowing systematic investigations of complex potential energy surfaces

[1] S. Furukawa & T. Komatsu, *ACS Catal.* 7 **2017** 735-765
[2] E. Gaudry *et al.*, *J. Mater. Chem. A* 8 **2020** 7422-7431
[3] B. Efron and T. Hastie, Computer age statistical inference, Cambridge University Press, **2016**

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**Location :**

The Institut Jean Lamour (IJL, Univ. Lorraine & CNRS) is a lab for fundamental and applied research in materials science; it brings together scientists from different disciplines. The LORIA (Laboratoire Lorrain de Recherche en Informatique et ses Applications, Univ. Lorraine & CNRS & INRIA) is a lab for basic and applied research in computer science. Both labs are located in Nancy (France), a nice city in the heart of Europe (close to Germany, Belgium, Luxembourg) and direct from Paris by TGV.

This project has an international dimension and takes place within the *Integrated European Center for the Development of New Alloys and Metallic Compounds (https://ecmetac.eu/)*, the research network *Open space between aperiodic order and physics & chemistry of materials* and the International Lab between IJL and the Joseph Stefan Institute (JSI, Ljubljana, Slovenia).