UNIVERSITÉ DE LORRAINE

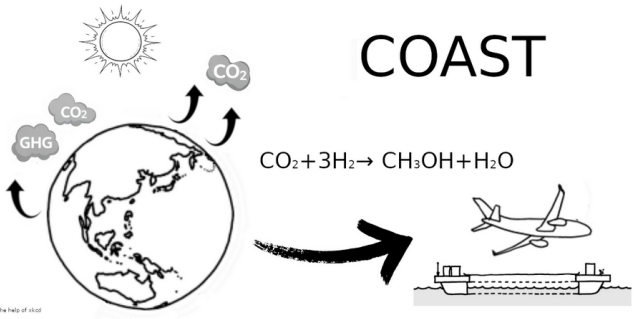
PhD position

Institut Jean Lamour
Campus Artem Nancy

LORIA
Campus Scientifique, Vandœuvre-lès-Nancy

Frugal Machine Learning and Density Functional Theory for the Design of Sustainable Catalytic Materials

Scientific context



The catalytic conversion of carbon dioxide into methanol is widely recognized as a key route for carbon valorization and greenhouse gas mitigation. When coupled with renewable hydrogen, this reaction offers a promising pathway toward sustainable fuel production and long-term decarbonization of the chemical industry. In recent years, catalysts based on oxide–metal and oxide–intermetallic interfaces have emerged as particularly promising systems, as these interfaces can strongly influence CO_2 activation and methanol selectivity. However, the atomic-scale structure of these interfaces and the mechanisms governing their catalytic activity remain poorly understood. Their structural heterogeneity and chemical complexity make accurate atomistic modeling particularly challenging.[1]

Recent advances in machine learning approaches provide a powerful framework to model complex catalytic materials with near *ab initio* accuracy while enabling simulations at significantly larger spatial and temporal scales than conventional electronic structure methods. However, these development typically requires very large training datasets generated from computationally expensive calculations, which represents a major bottleneck for the study of complex catalytic interfaces.

Objectives

The objective of the thesis is to develop data-efficient machine learning strategies for CO_2 hydrogenation to methanol, catalyzed by oxide-metal interfaces. Key ideas include the consideration of transfer learning, machine learning interaction potentials, and existing knowledge from experimental studies.

Techniques/methods in use: Density Functional Theory, Machine Learning

Applicant skills: Strong background in chemistry, physical chemistry, materials science, or condensed matter physics. Experience in data science, Python programming, high-performance computing and/or quantum chemistry will be considered an asset. Excellent communication skills are essential, with the ability to work and exchange ideas effectively both orally and in writing. English speaking is required. The application should include a statement of research interest, a CV and Master's degree transcript.

Supervisor(s):

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Internship location: IJL Nancy Campus Artem

[1] Hydrogen, Oxygen, and Lead Adsorbates on $Al_{13}Co_4$(100): Accurate Potential Energy Surfaces at Low Computational Cost by Machine Learning and DFT-Based Data, N. Boulangeot, F. Brix, F. Sur, and É. Gaudry, *Journal of Chemical Theory and Computation* **2024** *20* (16), 7287-7299