

BASF, Germany

IGSTC PhD Industrial Exposure Fellowship: Project Description

Title: Development and Application of Reactive Machine Learning Force Field for Complex Heterogeneous Catalysis

Description: Our proposal aims to develop and implement a reactive Machine Learning (ML) force field for complex heterogeneous catalysis applications. The foundation for this work has already been established by recent papers from our group, which demonstrate the feasibility and potential of using ML force fields in describing reaction networks for specific C1 chemistry. Our objective is to expand the protocol to include more complex and larger molecules, which are commonly found in industrial heterogeneous catalysis. By exploring the intricate surface and active site interactions, possibly with solvation effects, we aim to gain a deeper understanding of the underlying mechanisms and identify crucial performance-related descriptors.

One potential example application that we plan to focus on is the glycerol hydrodeoxygenation (DODH) reaction, which is of great industrial significance for the production of 1,3-propanediol. This reaction is a prime candidate for our study as it is a complex heterogeneous catalysis system that is of great industrial importance. A suitable candidate with appropriate skillset is expected to quickly get up to the speed in applying existing techniques and will be able to start making meaningful contribution in further development, which will ideally continue beyond the timeline of this internship.

***Minimum education and skillsets:**

- Currently enrolled in a Ph.D. program with focus on topics that include material science, catalysis, computational chemistry, machine learning etc.
- Demonstrated expertise in applications of quantum chemistry techniques (e.g., VASP, Quantum espresso etc.)
- Strong proficiency in python is must and familiarity with additional programming/scripting languages are desirable.
- Familiarity with machine learning algorithms.
- Familiarity with using scientific databases such as NOMAD, materials project etc. is desired.

*Kindly note that the skillsets required by BASF are over and above the eligibility criteria of IGSTC PhD Industrial Exposure Fellowships. PhD students who wish to get a Letter of Consent while applying to IGSTC Industrial fellowships are advised to contact BASF personnel if and only if they satisfy the above conditions.

Please send your resume and cover letter for this position to igstc.application@basf.com . Kindly note that an application without cover letter addressing skillset and motivation to join this project may be rejected without any notification.