



We create chemistry

IGSTC PhD Industrial Exposure Fellowship: Project I

Title: Integrated Data Management and Automation in Chemical Process Development

Description: The chemical processes for new active ingredients in the field of crop protection are developed in our department. During this development, data are generated in various formats, including chemical and engineering data from multiple sources. However, these circumstances often hinder efficient analysis and decision-making. The aim of this project is to improve the efficiency of chemical process development by seamlessly integrating diverse data formats, automating data transfer to machine-readable formats, and developing adaptable tools for automated data evaluation.

The methodology will involve developing algorithms to identify and normalize various chemical and engineering data, ensuring their compatibility. Additionally, scripts and protocols will be created to facilitate efficient transfer of integrated data to machine-readable formats. Further steps may include evaluating the data using process modelling tools. Programming languages such as Python or R may be used for practical implementation, but are not limited to these options. Once the methodology is realized, a validation phase will be conducted using real data from our process development team, encompassing both chemical and engineering data. At this phase, we plan to fine-tune and improve the functionality and performance of the tools especially considering user feedback. In summary, this project proposes a comprehensive approach to streamline data management in chemical process development, fostering efficiency and informed decision-making. To ensure the success of the project, the chemical process development team will provide the PhD student with the necessary support.

Minimum education and skillsets:

- Currently enrolled in a PhD program with focus on chemical engineering topics.
- Knowledge of data management and design of experiments.
- Familiarity with programming languages like python or R is desirable.
- Experience with thermodynamic simulation programs and substance property data tools.

*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 with "IGSTC Industrial Fellowships 2024" in the subject of the email. Kindly note that an application without cover letter addressing skillset and motivation to join this project may be rejected without any notification.



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IGSTC PhD Industrial Exposure Fellowship: Project II

Title: Development and Application of Organocatalytic Transformations in an Industrial Setting

Description: We are looking for a highly motivated candidate to join our Group "Cross Indication Synthesis" within the Agricultural Solutions business unit. In this role, you will play a crucial part in the development of industrially relevant chemical transformations, focusing on achieving synthetic excellence. Recently, we have conceptualized new organocatalytic reactions to access key intermediates within the synthesis of biologically active ingredients. Preliminary in-house results serve as foundation to develop widely applicable chemical transformations in an industrial setting. Your responsibilities will include optimizing these reactions and investigating their applicability as a general tool in chemical synthesis. Furthermore, you will have the opportunity to utilize these newly developed strategies in the synthesis of biologically active compounds, potentially contributing to the development of the next generation of crop protection products.

Additionally, the candidate will work on the implementation of asymmetric Organocatalysis as a tool to synthesize enantiomerically enriched building blocks, specifically those, which remain challenging to access with conventional methods. In this context, the candidate will systematically investigate a variety of reaction conditions in the presence of several enantiomerically enriched organocatalysts. The candidate is expected to organize, analyze, and interpret the generated data set and ideally suggests follow-up steps in a proactive fashion.

Minimum education and skillsets:

- Currently enrolled in a PhD program that include organic synthesis, preferentially with focus on method development, stereoselective catalysis or total synthesis.
- Intrinsic self-motivation and ability to work independently.
- Passionate about synthetic organic chemistry and proactive in implementing creative ideas.
- Deep knowledge of EHS requirements within synthetic laboratories.
- Excellent organizational skills and ability to thrive in an international environment.

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IGSTC PhD Industrial Exposure Fellowship: Project III

Title: Application of Interface Force Field model of metal oxides for the surface pretreatment technology

Description: We are looking for a highly motivated candidate to join our Group “Molecular Modeling & Drug Discovery” within the Group Research division. In this role, you will play a crucial part in the development of industrially relevant chemical transformations, focusing on achieving sustainable surface pretreatment technology for metal oxide and recycled alloy surfaces in automotive, aerospace & construction industries among others. Using molecular modeling we are trying to predict how metal oxides will react with different pretreatment chemicals. Recently, we have developed the Interface Force Field (IFF) model to design new surface pretreatments that are more effective and environmentally friendly.

Your responsibilities will include optimizing all-atom models of metal oxide surfaces to perform accurate MD simulations of surface interactions in electrolytes at various pH values. The models should be able to predict the adsorption behavior of different polymers on various metal oxide surfaces, which is crucial in designing effective coatings. Additionally, you will learn how to use the LAMMPS workflow in combination with the EMC (Enhanced Monte Carlo Structure Generator) software (<https://montecarlo.sourceforge.net/emc/Welcome.html>), umbrella sampling using SSAGES and create the coarse-grain parameterizations for metal oxide-organic interface.

Minimum education and skillsets:

- Currently enrolled in a PhD program that include materials molecular modeling, preferentially with focus on all-atom force field development, computation of adsorption free energy and exposed to coarse-grained MD simulations.
- Familiar with Linux OS, MD simulations using LAMMPS, Data analysis, Python programming.
- Intrinsic self-motivation and ability to work independently.
- Passionate about interfacial chemistry and proactive in implementing creative ideas.
- Excellent organizational skills and ability to thrive in an international environment.

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