IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Development of nanostructured carbon supports and nanocatalysts for sustainable heterogeneous organic catalysis**
Project Number	**IMURA0853** BASF We create chemistry

Monash Main Supervisor (Name, Email Id, Phone)	Prof. Alan Chaffee Alan.chaffee@monash.edu	*Full name, Email*
Monash Co-supervisor(s) (Name, Email Id, Phone)		
Monash Head of Dept/Centre (Name,Email)	Prof. Phil Andrews phil.andrews@monash.edu	*Full name, email*
Monash Department:	School of Chemistry	
Monash ADRT (Name,Email)	Prof. Peter Betts (peter.betts@monash.edu)	*Full name, email*
IITB Main Supervisor (Name, Email Id, Phone)	Dr. C. Subramaniam csubbu@chem.iitb.ac.in	*Full name, Email*
IITB Co-supervisor(s) (Name, Email Id, Phone)		*Full name, Email*
IITB Head of Dept (Name, Email, Phone)	Prof. Anindya Datta anindya@chem.iitb.ac.in	*Full name, email*
IITB Department:	Chemistry	

Research Clusters:	**Research Themes:**
Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST* ***one.*** *For more information, see www.iitbmonash.org)*	**Highlight which of the Academy's Theme(s) this project will address?** *(Feel free to nominate more than one. For more information, see www.iitbmonash.org)*

1	*Energy, Green Chem, Chemistry, Catalysis, Reaction Eng*	***1***	*Nanotechnology*

The research problem

Heterogeneous organic catalysis, such as hydrogenation of olefins and related organic compounds, forms a fundamentally important and industrially critical process for applications ranging from pharmaceuticals to fuels. Heterogeneously catalyzed reactions offer distinct advantages in terms of product recovery and purification. However, the reaction rate is often mass-transfer limited due to the phase-difference between the reactants (liquids or gases) and the catalyst (solid). Overcoming mass-transfer limitations can lead to adverse effects on selectivity of reaction leading to unwanted by-products. Further, the lifetime, recyclability and atom efficiency of the heterogeneous catalyst is strongly dependent on the fundamental surface interactions between the support and catalyst. The high temperatures and pressures employed in such reactions can often lead to aggregation (sintering) of catalysts over the support surface leading to degradation of the catalytic activity. Well dispersed metal nanoparticles are generally the preferred form for the active catalysts, yet insufficient attention has been devoted to the development of synergistic catalytic supports. Herein, the surface energy of the catalyst nanoparticle on the surface of support is vital to prevent aggregation of catalyst. The uniform distribution of catalyst nanoparticles over a high-surface area, porous support is critical to achieve industrially sustainable catalysis. This ensures the optimal orientation of the active surface of catalyst towards the reactant and simultaneously provides facile access of the active site to the reactant. This research activity aims to develop a fundamental understanding of the support-catalyst interactions, for specific organic hydrogenation reactions, by employing a combination of both in-situ and ex-situ spectroscopic and microscopic techniques. The knowledge thus generated will be used to engineer nanostructured carbons and carbon monoliths as synergistic support for heterogeneous catalytic reactions.

Project aims

1. *Development of nanostructured carbon materials and carbon monoliths with the optimal combination of surface area, porosity, thermal-stability, chemical-stability and mechanical durability as supports for organic hydrogenation reactions*
2. *Development of processes for optimal and uniform loading of catalysts nanoparticles over such supports.*
3. *Understanding of support-catalyst interactions through a combination of in-situ and ex-situ spectroscopic and microscopic techniques.*
4. *Evaluation of such synergistic carbon supported catalytic systems for organic reactions of industrial relevance (ex. hydrogenation of olefins)*

Expected outcomes

Besides providing a fundamental understanding of the support-catalyst interactions, the study is expected to advance the development of novel nanostructured carbons and carbon monoliths for heterogeneously catalysed olefin-hydrogenation reactions. The lifetime of the support-catalyst systems developed would be benchmarked against conventionally available materials and processes against parameters of surface area, porosity, thermal stability, mechanical robustness and catalytic performance.

How will the project address the Goals of the above Themes?

The project relates to the Theme of Chemical catalysis and seeks to develop nanomaterials based heterogeneous catalytic systems for achieving sustainable industrial process.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

Masters/M.Tech in Chemistry with expertise in both fundamental and application-oriented aspects of Chemistry and Chemical Engineering.
Analytical and lateral-thinking ability
Skill in tooling for fabricating custom-built metal-based components is an added advantage.

Potential Collaborators

Industrial collaboration with BASF

Major Milestones:

Please add major intended milestones for the project

#	Milestone	Deliverable	Timeline	Responsible
A	• Literature review on	• Existing approaches for	6 months	IITB

	catalysts and carbonaceous supports for hydrogenation catalysts.	heterogeneous organic reactions and their disadvantages. • Properties required for catalyst and support to provide atom-efficient catalysis		
B	• Fabrication of nanostructured carbon supports • Development and characterisation of catalyst loaded supports	Initial results for thermal, chemical and mechanical stability of catalyst-loaded supports.	12 months	IITB
C	• Design of "model" catalyst-support systems based on fundamental investigation into catalyst-support interactions	Fundamental understanding of catalyst-support-reactant interactions. New directions to improve catalytic efficiency	18 months	IITB
D	• Iterative experiments to tailor and tune catalyst-support systems. • Optimisation of reaction conditions.	Optimising catalyst using a series of tailored nanostructured carbon-based supports and monoliths.	24 months	IITB + Monash
E	• Testing stability and performance of catalytic systems	Understanding parameters influencing catalytic efficiency and means to optimise them.	36	IITB + Monash
F	• Preparation of manuscripts and patents • Compilation of results in the form of thesis	Intellectual property with potential commercial implications. Scientific publications in international, peer-reviewed journals with high impact.	48 months	IITB + Monash