IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Predicting separation selectivity in nanoporous materials**
Project Number	**IMURA0356**

CSIRO

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Research Academy Themes:

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. **Advanced computational engineering, simulation and manufacture**
2. Infrastructure Engineering
3. Clean Energy
4. Water
5. **Nanotechnology**
6. Biotechnology and Stem Cell Research

The research problem

Define the problem

Hydrogen is considered as an alternate fuel source suitable to replace natural fossil fuel resources. However, a vast majority of hydrogen is produced from syngas, which are typically a mixture of a large number of gases, including hydrogen and carbon dioxide. Separation of gas mixtures, particularly the separation of carbon dioxide from other gas mixtures is an important industrial problem. To purify hydrogen, carbon dioxide separation from syngas is a prerequisite. Moreover, carbon dioxide is a green house gas, and therefore its separation and sequestration is also crucial for on-site environmental protection for power plants, where majority of flue gas is emitted. Several techniques are proposed to

separate carbon dioxide from gas mixtures and among these, adsorption in porous materials is economically competitive.

In this project, in combination with experimentalists at the Commonwealth Scientific and Industrial Research Organisation (CSIRO), we aim to develop this fundamental understanding of this very applied research problem using the state-of-the-art computational techniques.

Project aims

Define the aims of the project

1. To provide new insights into the microscopic properties of guest molecules in porous materials. Guests confined in porous materials behave differently from bulk phases and quantitative understanding at the molecular scale is indispensable.
2. To predict structure-function relations from bottom up for the intelligent design of porous materials with desired architectures and functionalities.
3. To predict structural, thermodynamic properties and adsorption selectivity based on Monte Carlo simulations.

Expected outcomes

Highlight the expected outcomes of the project

This project is expected to provide new knowledge for the molecular design and screening of porous materials for separation applications. Moreover, modelling studies can provide microscopic insight and complement experimental studies.

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

1. This project involves multi-scale simulations requiring high-performance computing to design and screen different porous materials, and hence is aligned with the theme of Advanced Computational Engineering, Simulation and Manufacture.

2. The key structural features and the molecular phenomena of the porous materials of interest are essentially nano-scale and impact the overall macroscopic performance. Thus tailoring the structure at the nano-scale is a major aspect of this project and makes it highly relevant for the theme of Nanotechnology.

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.

i) B.Tech/M.Tech degree in Chemical Engineering or other engineering disciplines
ii) M.Sc. in Physics or Chemistry

Capabilities: An ideal candidate will have a strong interest in computational studies of nanoscale materials. The candidate with some experience and interest in basic programming languages (Fortran/C/C++/MATLAB) will be preferred