

An Indian-Australian research partnership

**Project Title:** Development of photothermal catalysts for sustainable carbon dioxide conversion using solar energy.

**Project Number** IMURA1091

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## Research Clusters:

## Research Themes:

Highlight which of the Academy's CLUSTERS this project will address? (Please nominate JUST <u>one</u> . For more information, see <a href="http://www.iitbmonash.org">www.iitbmonash.org</a> )		Highlight which of the Academy's Theme(s) this project will address? (Feel free to nominate more than one. For more information, see <a href="http://www.iitbmonash.org">www.iitbmonash.org</a> )	
1	Material Science/Engineering (including Nano, Metallurgy)	1	Artificial Intelligence and Advanced Computational Modelling
2	Energy, Green Chem, Chemistry, Catalysis, Reaction Eng	2	Circular Economy
3	Math, CFD, Modelling, Manufacturing	3	Clean Energy
4	CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control	4	Health Sciences
5	Earth Sciences and Civil Engineering (Geo, Water, Climate)	5	Smart Materials
6	Bio, Stem Cells, Bio Chem, Pharma, Food	6	Sustainable Societies
7	Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng	7	Infrastructure
8	HSS, Design, Management		

## The research problem

### *Define the problem*

The concept of converting CO<sub>2</sub> into synthetic fuels and chemicals using sunlight as the sole energy source holds tremendous prospects for establishing a sustainable carbon-neutral economy. Unfortunately, the light utilization efficiency of CO<sub>2</sub> conversion via traditional photocatalytic processes, that utilize only UV/purple light, remains too low for practical use. "Photothermal" catalysis is an emerging field that employs plasmonic materials to utilize the full spectrum of sunlight (UV, visible, and IR spectra) and can combine both thermal and photochemical contributions of sunlight to drive catalytic reactions at unprecedented rates.

However, the research area is new, and catalyst development for photothermal CO<sub>2</sub> conversion remains in an under-utilized and rudimentary stage. The choice of appropriate catalysts is critical to ensure effective combination of light and heat to achieve practically relevant product yields under realistic sunlight conditions. Photothermal conversion of CO<sub>2</sub> is a multi-step and multi-functional process, with various functional sites operating in tandem to harvest light and photothermally convert CO<sub>2</sub>. Intricate design and engineering of the catalyst structure and morphology at the nano scale is required to maximize the synergetic functioning of the various functional sites.

The proposed research aims at developing tailor-made photothermal catalysts for light-driven CO<sub>2</sub> hydrogenation to solar methane by engineering hierarchical carbon-containing nanostructures derived from metal organic frameworks (MOFs), that can facilitate synergistic functions of light harvesting, photon-to-heat conversion, heat retention, and CO<sub>2</sub> activation. A primary focus of catalyst synthesis and development would be to study the effect of catalyst morphology on photothermal activity and to develop rigorous structure-property relations that can be used to develop catalysts with high solar-to-fuel conversion efficiency.

The scientific outcome of this research can result in significant technical advances in the sustainable and renewable conversion of CO<sub>2</sub> to fuels and valuable products.

## Project aims

### *Define the aims of the project*

The overall aim of the project is to develop active and stable catalysts that can absorb sunlight and photothermally generate energetic electrons and localized heat to convert CO<sub>2</sub> to methane, without the requirement of any external heat supply.

The main objectives of this project are:

1. To develop effective multi-functional catalysts with hierarchical architecture incorporating plasmonic nanomaterials in carbon frameworks for photothermal CO<sub>2</sub> hydrogenation to methane.
2. To develop structure-property relations between catalyst morphology /composition and catalytic activity in photothermal CO<sub>2</sub> hydrogenation to methane.
3. To determine mechanistic contributions of thermal and electronic excitation effect of light in the catalysis, and to apply these insights to optimize catalyst design and reactor operating conditions.

## What is expected of the student when at IITB and when at Monash?

### *Highlight how the project will gain from the students stay at IITB and at Monash*

#### At IITB:

- Conduct experiments to synthesize hierarchical carbon-containing photothermal catalysts using metal-organic frameworks to host plasmonic and catalyst metal nanoparticles.
- Characterize the synthesized catalysts using techniques such as TEM, XRD, TPDRO, XPS, BET, UV/Vis, FT-IR spectroscopy to determine morphology, optical, and physicochemical properties.
- Study the catalytic performance of the synthesized catalysts in photothermal CO<sub>2</sub> hydrogenation.
- Study the effect of modulation of the catalyst morphology and composition on its photothermal activity.
- Conduct control experiments varying light intensity and wavelength to determine the dominant pathway for photothermal CO<sub>2</sub> activation (plasmonic heating vs. hot electron chemistry).

#### At Monash:

- Conduct advanced characterization of photothermal catalysts using XAS to determine electronic and geometric state of active metals.
- Conduct operando spectroscopic studies (such as *in situ* DRIFTS and XAS) to gain insights into reaction mechanism and key reaction intermediates.
- Interpret spectroscopic characterization data vis-à-vis reaction performance to hypothesize structure-property relations for future catalyst development.

## Expected outcomes

*Highlight the expected outcomes of the project*

The expected outcome of the proposed research include:

- The development of new and efficient catalysts for the photothermal conversion of CO<sub>2</sub> to methane using light as the only source of energy.
- Scientific understanding of the interaction between light, photo-generated heat, catalytic sites, and reaction pathways for CO<sub>2</sub> conversion, which can lead to improved rational designs of photothermal catalysts with higher solar-to-fuel conversion efficiencies.

The proposed research can lead to outstanding technological advancements in the field of solar-driven sustainable catalytic conversion of CO<sub>2</sub> to fuels, that can address critical issues related to energy and environment globally.

## 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.*

The proposed project on the catalytic conversion of CO<sub>2</sub> to hydrocarbons on Mo<sub>2</sub>C is expected to address the goals of clean energy, smart materials, and advanced computational modelling themes in the following ways:

- **Clean Energy:** The project aims to develop effective catalysts for converting CO<sub>2</sub> to fuels using renewable solar energy. In contrast to thermal routes of CO<sub>2</sub> conversion that depend on external fossil-fuel derived energy to drive the reaction, photothermal catalysts have the potential of converting CO<sub>2</sub> in a truly sustainable way without causing excess carbon emissions. With the right choice of catalysts, photothermal processes can also potentially achieve product yields that are several orders of magnitude higher than what can be achieved by traditional photocatalysis. Thus, the scientific and technological advances from this proposed research can contribute tremendously towards the goal of clean energy and environmental sustainability.
- **Circular economy:** Capture and recycle of CO<sub>2</sub> to produce fuels and chemicals forms an important part of the concept of a circular carbon economy. By developing catalytic materials and processes that can conduct the conversion of CO<sub>2</sub> through the use of renewable solar energy, this research further attempts to reduce greenhouse gas emissions in the process of CO<sub>2</sub> recycling and reuse.
- **Smart Materials:** The project aims to design, synthesize, and optimize novel MOF-derived catalytic materials with advanced nano-architectures for the solar-driven conversion of CO<sub>2</sub> to fuels. The ideal catalytic material for this conversion should be able to absorb the entire range of sunlight, generate and retain photo-induced heat, and effectively channel photo-generated charges and electrons to the reactants and reaction intermediates to convert CO<sub>2</sub> into fuels without any external heat consumption. The simultaneous and synergistic occurrence of all these functionalities requires intricate design of novel functional materials. This study aims at the nano-scale design and synthesis of such functional and smart materials, that can effectively harness solar energy to drive chemical transformation of CO<sub>2</sub> to fuels.

## Potential RPCs from IITB and Monash

*Provide names of the potential research progress committee members (RPCs) and describe why they are most suited for the proposed project*

IITB:

- Prof. Sanjay Mahajani
- Prof. Arindam Sarkar

Monash:

- Prof Paul Webley
- Prof Sankar Bhattacharya

## 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.

Undergraduate in Chemical Engineering or in Chemistry.

Knowledge of chemical reactions, reaction kinetics.

## Necessary Courses

Name three tentative courses relevant to the project that the student should complete during his/her coursework at IITB (the student will require to secure 8 point in these courses)

CL 605 Advanced Reaction Engineering

CL 601 Advanced Transport Phenomena

CH 547 Organometallic Chemistry/Catalysis

## Potential Collaborators

Please visit the IITB website [www.iitb.ac.in](http://www.iitb.ac.in) OR Monash Website [www.monash.edu](http://www.monash.edu) to highlight some potential collaborators that would be best suited for the area of research you are intending to float.

Select up to **(4)** keywords from the Academy's approved keyword list (**available at <http://www.iitbmonash.org/becoming-a-research-supervisor/>**) relating to this project to make it easier for the students to apply.

- Catalysis and reaction engineering
- Novel functional materials
- Green chemistry and renewable energy
- Nanotechnology/ nano-science