

An Indian-Australian research partnership

Project Title: **Functional Coordination Networks and Cages for Molecular Applications**

Project Number **IMURA0372**

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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

The research project will simultaneously address two issues, namely the storage and activation of small molecules. There is a considerable research drive towards molecular recognition of small molecules using either homogenous or heterogeneous host species. The ability to selectively target specific molecules has potential applications in:

- Storage of gas molecules for energy applications.
- Protection of highly reactive species from bulk media.
- Stabilization of otherwise unstable species inside the host
- Targeted delivery of therapeutic molecules.
- Catalysis within nanoscale molecular reaction vessels.
- Separation of complex mixtures.
- Remediation of environmental pollutants or biological toxins.

The problem to be overcome is the deliberate design of either discrete molecular cages or porous materials that contain the correct pore size, geometry and chemical functionalities to be able to act as effective and selective hosts towards small molecular guests. The use of coordination chemistry in self-assembling systems provides a means of designing and synthesising such materials using tailored ligands to enforce the desired molecular architectures. Judicial choice of chemical functionalities and metal ions has the potential to tailor the behaviour of the resulting materials/cages.

Project aims

The overarching aim of the project is to utilise coordination polymers and nanoscale coordination cages to produce novel materials that are capable of encapsulating, detecting or catalysing the reactions of small molecules. The emphasis will be placed on small molecules/ions with important environmental, biological or industrial applications with the aim of improving existing methods of detection, remediation or synthesis.

The project will proceed in three main sections:

- Synthesis of organic ligands: Novel organic species will be designed that have the capacity to bridge between metal ions. These will incorporate coordinating functionalities such as carboxylic acids, imidazole, pyridyl and other N-heterocycles. One of the main aims of the project will be to incorporate an additional functional site to the 'interior' of the ligand to provide a site at which guest species can interact, thereby imparting selectivity on the resulting coordination complexes. Initial target species will be symmetrically functionalised molecules with work progressing towards heterotopic species (with different coordinating groups at each end) which provide a more novel route towards interesting materials.

- Synthesis and analysis of coordination cages / polymers: Once synthesised, the organic ligands will be incorporated into metal-organic systems with careful screening of reaction conditions to drive the self-assembling system towards different products. A variety of methods will be employed towards these goals including solvothermal synthesis (at elevated temperatures and pressures) with early transition metals and more traditional coordination chemistry involving noble metals and platinum group metals. The aim will be to template the ligands into forming porous materials or coordination complexes that contain a large internal space.

- Study of guest behaviour and physical properties: The porous materials/complexes that are obtained will be tested to explore their behaviour in the presence of small guest species. The target guests are environmentally important gases (H_2 , CO_2), small chiral molecules (to test enantiomeric selectivity if chiral ligands are used), small reactive species (to see if reactivity can be controlled within the confines of the materials) and small cationic/anionic species (particularly those of environmental or biological significance).

Throughout the project, an ongoing and important aim will be to understand the processes of formation behind the self-assembly in these new systems and tailor subsequent synthesis according to this new understanding.

Expected outcomes

The outcomes of the research will be:

- Novel cage complexes that are capable of stabilising reactive molecules and/or of displaying selective recognition in solution. Uses of these compounds will be fully explored, including examining the lifetimes of host-guest species, exploration of selectivity against similar species and the potential for slow release of guests.

- Porous coordination polymers (MOFs) that are capable of displaying significant gas uptake and/or that show selectivity in the removal of species from solution. Guest adsorption will be examined in detail to understand how the materials function with a view to using this knowledge for latter generation materials.

- Fundamental advances in the understanding of self-assembly as a mechanism for synthesising both discrete and extended coordination complexes. Structural studies will be under-taken on a wide range of materials to explore the interplay between different classes of interactions in order to develop more robust or directed self-assembling systems.

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

The project will address two of the academy themes:

- 3, Clean Energy: Porous materials, comprising either coordination polymers or tightly packed porous cages, will be explored for their applications in the storage of gases such as H_2 and CO_2 . Safe storage of hydrogen gas under conditions that approach ambient remains a major obstacle for the use of hydrogen as a fuel in transportation. There is a need for lightweight materials that adsorb significant amounts of H_2 without the need for high pressures or cryogenic temperatures. Carbon dioxide is also a major target species as rising levels of this gas, from anthropogenic emissions, are largely thought to be responsible for climate change. The ability to sequester CO_2 from industrial gas flues would enable carbon capture and storage processes to reduce the amount of gas reaching the atmosphere. The porous materials that are the aims of this project have the potential to adsorb these gases, amongst others, and tailoring materials to be selective towards guests that are of importance for clean energy is a key aim of the research.

- 5, Nanotechnology: The materials that will be synthesised will be designed to have nanoscale porosity, i.e. the interior of cages and the internal diameter of porous coordination polymers will typically lie in the range 1 – 2 nm. These materials, if appropriately functionalised, have the potential to be tethered to surfaces to create functional surfaces with nanoscale pores. Depending on the surface that is used this can lead to detection devices or separation membranes using the coordination complexes as the functional nanomaterial.

Capabilities and Degrees Required

- *A first-class undergraduate degree in Chemistry (MSc) or a closely related discipline.*
- *Experience of laboratory-based research (i.e. undergraduate / MSc research project).*
- *A demonstrated passion towards chemical research.*