

An Indian-Australian research partnership



**Project Title:** Novel methods for high throughput experimental materials design optimisation

**Project Number** IMURA0206

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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](http://www.iitbmonash.org))*

1. Advanced computational engineering, simulation and manufacture

## The research problem

*Define the problem*

Development of a new material, product, process or technology often depends on experimental optimisation of component combinations and/or processing parameters. Current advances in high throughput experimentation methodology allow this experimentation to be increasingly thorough, expanding the domain of possible response behaviour surveyed beyond the limits of application of many classical techniques for experimental design and analysis.

The objectives of this project are therefore to:

1. Compare a number of approaches including classical DoE, various stochastic approaches (for example, evolutionary or Monte Carlo techniques) and space-filling methods, noting in particular their sensitivity to the special features characteristic of high throughput combinatorial experimentation:
  - sequential batch experimentation;
  - gradient techniques (where varying proportions of ingredients are mixed in a continuous, non-random manner);
  - the presence of experimental error;
  - objective function evaluations (primarily material property measurements) that may still be relatively expensive;
  - the possibility of complex response surfaces which may not be able to be described by low order global parameterisations.

2. Develop a suitable methodology for design and analysis of modern high throughput experiments.

3. Create software implementing the new methodology.

The strategy to be followed will largely consist of computer simulation techniques (ideally a suitable physical materials development programme can be found on which to validate the methodology; this depends on funding and opportunities and is not fundamentally necessary for the scope of the PhD studies). The various methodologies can be implemented and tested on some standard simulated materials development models in the literature, expanded as necessary.

### **Expected outcomes**

*Highlight the expected outcomes of the project*

1. Development of methodology appropriate to high throughput experimental materials development.
2. Insight into optimisation and search methods and development of adaptations that improve their application to problems of this type.
3. Creation of software using new methodology to generate experimental designs (and perform analysis of results where this is non-standard), either as a stand-alone product or within an environment like R or Excel (which is more accessible for end users). The final form of this software will depend on the requirements of the approach chosen.