## MONASH ENGINEERING



# Faculty of Engineering Summer Research Program 2022-2023

Project Title: Designing Magnetism in 2D Materials

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#### Objective

This project will investigate magnetism in novel 2D materials for applications in electronic and spintronic devices. For this computational project, you will employ modern computing tools on massively parallel computing systems and learn highly employable skills such as advanced computing, modelling and data analysis.

### **Project Details**

Two-dimensional (2D) materials have applications in future low-energy electronics. One way to realise 2D materials is with metalorganic frameworks, which combine transition metal ions with organic molecules to create a crystal structure. This computational project will investigate different 2D metal-organic frameworks for evidence of strong electronic interactions. The effect of changing ligands, metal atoms, and lattice geometries will be explored. This will build a catalogue of interesting materials for experimental study and discover trends relating the physical features to the electronic parameters. This project will use state-of-the art software packages and massively parallel highperformance computing clusters.



#### Prerequisites

An avid interest in computer simulations