



**UNSW**  
SYDNEY



## PhD in Nanomaterials Data Science

**Details:** The Faculty of Engineering at the University of New South Wales in Sydney, Australia, has an opening for a PhD student in the field of Nanomaterials Data Science, in collaboration with Dr Amanda Barnard at CSIRO Data61. The position is for a term of 3.5 years, and commences as soon as possible, with a stipend of \$27,596 per annum with all tuition fees covered by the university. The possibility of a further “top-up” scholarship is available, depending on the credentials of the candidate.

### **Project: Data Science for Solving the Synthesis-Structure-Function Relationships Problem for Multimetallic Nanocatalysts**

This project aims to use computational modelling and data science, coupled synchrotron radiation characterization methodologies, to solve the synthesis-structure-function relationship problem for multimetallic nanocatalysts. The combination of multiple metal species within a single catalyst often leads to synergistic enhancements in catalytic properties (reactivity, longevity, selectivity and/or cost). As all “as-synthesized” nanoparticles include heterogeneous sizes and structural defects, many discoveries to date are made serendipitously without understanding how atomic scale structure can be tuned by synthetic conditions or how the resulting structures influence catalytic properties. To date, all efforts to develop the requisite fundamental knowledge are often done on a “case by case” basis, wherein a hypothesis is tested against a small set of samples and conditions with the goal of understanding key fundamental knowledge to help improve catalytic performance. The rate to which this loop is completed is often limited by the bandwidth of the experimenter(s) and requisite time needed to develop meaningful observations.

The incorporation of data science aims to enhance such processes by pulling from rich datasets generated from such experiments to increase meaningful discoveries in catalysis. The ability to tune multimetallic nanoparticles in composition, size and surface ligand provides a strong starting basis of data ripe for high throughput synthesis. Subsequent structure modelling, built from one or more synchrotron characterization datasets, provides atomic coordinates and chemistry ripe for data science analytics, while catalytic outcomes provide an end goal metric for dictating future materials development.

**Location:** This project is a collaborative effort between Data61 at CSIRO and UNSW, and will be based at Data61 in Melbourne, Australia, with Dr Amanda Barnard; as the prospective student will focus heavily on the data science methodologies. Participation in synchrotron experiments (also based on Melbourne, Australia) is optional, albeit a useful endeavour that does not require much experience in chemistry.

**To apply:** Prospective students are encouraged to contact Dr. Nicholas Bedford ([n.bedford@unsw.edu.au](mailto:n.bedford@unsw.edu.au)) at their earliest convenience.

**Open until filled.**