**University of Leicester**

**Future 50 PhD Scholarship**

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| **Project Reference** | Chem Cao |

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**Section 2 – *Project Information***

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| **Project Title** | Sustainable synthesis of *N*-heterocycles using single atom catalysts (SACs) via oxidation reactions |
| **Project Highlights:** | 1. | Catalytic methodology development: Sustainable synthesis of high value-added *N*-heterocycles produced from widespread bulk chemicals via oxidations using heterogeneous single atom catalysts (SACs). |
| 2. | Organic synthesis: Evaluation of catalytic properties of SACs towards oxidation reactions using gas/liquid chromatography (GC and HPLC), and characterization of isolated *N*-heterocycle products using IR, UV-vis and NMR spectroscopy. |
| 3. | Functional nano-materials synthesis and characterization: Synthesis various of SACs and characterise their atomic morphology and active sites using modern characterization techniques for nano/porous materials (e.g., SEM, STEM, XPS. XAS, BET, TGA).  |
| **Project Summary**  |
| **Introduction**Selective oxidation is an important strategy for producing valuable compounds range from kilogram-scale fine chemicals in pharmaceuticals to kiloton scale in bulk chemicals. However, compared to hydrogenation, oxidation is underdeveloped. Traditional catalytic routes generally use expensive homogeneous transition metal complexes with non-environmentally friendly oxidants, which poses a challenge to sustainability and separation/recycling of the catalyst. With the rapid growth of nanoscience, heterogeneous catalysts, mainly supported transition metal nanoparticles, have been exploited to tackle these problems; however, their overall catalytic efficiencies are usually inferior to their homogeneous counterparts with lower selectivity and require harsh reaction conditions. Single-atom catalysts (SACs) are defined as catalyst in which the active metal species exist as isolated single atom stabilized by the support or by alloying with another metal.1 When considering the supports as rigid ligands from the viewpoint of coordination chemistry, SACs can serve as a bridge between homogeneous and heterogeneous catalysts and have the possibility of integrating the merits of both types of catalysts.2 **Project Outline**This project aims to develop SACs with superior performance to well-established catalytic systems, and to exploit their inherent attributes to revolutionise chemical synthesis by creating new sustainable synthetic strategies for *N*-heterocycles. Success in the area will allow high value-added *N*-heterocycles produced from widespread bulk chemicals, reduce energy consumption and decrease environmental pollution attributed to hazardous oxidants. Two aims are outlined:1. Develop a new sustainable catalytic method for *N*-heterocycles synthesis via oxidation of C-H bonds/alkenes using *N*-doped carbon supported SACs.
2. Synthesis various of *N*-doped carbon supported SACs with non-noble metals. To guide the rational catalyst design, the activity and physical /chemical structures of *N*-doped SACs will be investigated using kinetic analysis and modern characterization techniques for nanomaterials and porous materials.

Applicants for this PhD need to have an interest in synthetic organic chemistry and functional nanomaterial manufacturing & characterisation. Successful candidate will gain extensive experience in organic synthesis, analytical methods (e.g., GC-MS, HPLC, UV-vis, IR, NMR) and modern characterization techniques for nano/porous materials (e.g., SEM, TEM, STEM, XAS, BET, TGA). 1. Acc. Chem. Res. 2013, 46, 8, 1740–17482. Nat. Rev. Chem, 2018, 2, 65-81. |