

**GTA Studentship for September 2024 entry**

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| **Scheme:** | **School of Chemistry Graduate Teaching Assistant (2024 Entry)** |

**Mechanochemical synthesis for sustainable chemical manufacturing**

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| **Project Title** | Mechanochemical synthesis for sustainable chemical manufacturing | |
| **Project Highlights:** | 1. | Solvent-free methods applied to chemical synthesis |
| 2. | Earth-abundant metals as alternatives to expensive critical materials |
| 3. | Reactivity with strategic industrial feedstocks – H2, CO, CO2 and N2 |

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| **Project Summary** |
| ***Background***  There is an urgent need to break our reliance on precious metals (e.g. Pd, Pt) in the chemical industry owing to their scarce availability, high costs and sustainability concerns. AE alkaline earth metals are very environmentally benign and cheap (Mg £2/kg, Ca £2/kg, Ba £20-50/kg); crucially, low-valent AE metals possess physicochemical properties suitable to replace precious metals, modernise and improve efficiency in the chemical industry, as they have already shown great potential in the activation of small molecules of great relevance for chemical engineering applications (*e.g.* N2, Haber-Bosch; CO/H2, Fischer-Tropsch). Despite their great promise, their applications have been blocked by the challenging preparation of low-valent AEs.  ***The Project***  This project aims to address key issues which threaten the long-term sustainability of chemical engineering and manufacturing. The PhD candidate will deliver the first facile synthesis of low-valent AE electrides (i.e. materials where electrons are delocalised and not associated with well-defined sites/atoms) and unlock their application as earth-abundant alternatives to precious metals that will transform the chemical industry. The work will be based on the innovative use of mechanical forces (i.e. mechanochemistry) developed by the Ortu Group, in which we have shown that simple AE amide precursors (e.g. [Ca{N(Mes)(SiMe3)}3K] can be converted into highly reactive AE electrides (**I**, Figure 1) *via* quick solvent-free synthesis with minimal manipulations; these species are able to perform facile C-H activation chemistry and pyridine coupling (work currently under consideration with *Nature Communications*). Crucially, our mechanochemical methods can significantly reduce the use of hydrocarbon solvents and deliver quick and scalable multi-gram synthesis under very mild conditions. The PhD candidate will be to build on these exciting preliminary results by developing new AE electrides and targeting strategic reactions for the chemical industry and fine chemical production (*e.g.* Fischer-Tropsch, Haber-Bosch, C-C coupling).  AE electrides will be synthesised using mechanochemical methods, supported by state-of-the-art anaerobic techniques (Schlenk line and glovebox), advanced organometallic and organic synthesis. The student will be involved in the physical characterisation of the new materials (EPR, electron-conductivity, XRD, XAS, RINXS) working alongside national and international collaborators.    ***Figure 1:*** *Synthesis of a Ca electride (****I****) and its reactivity.* |

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**See the GTA web page for application advice and link to the online application**