**University of Leicester**

**Future 50 PhD Scholarship**

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| **Project Reference** | CHEM Rodriguez Macia |

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| **First Supervisor** | Dr Patricia Rodriguez Macia  |
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| **Additional Supervisor** |  |

**Section 2 – *Project Information***

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| **Project Title** | Engineering CO Dehydrogenase Enzymes: Toward Artificial Metalloenzymes for efficient CO2 reduction |
| **Project Highlights:** | 1. | Artificial Metalloenzymes for CO2 conversion |
| 2. | Genetic engineering of metalloenzymes |
| 3. | Evaluation of the catalytic properties of artificial metalloenzymes by electrochemical and spectroscopic techniques |
| **Project Summary**  |
| Global warming caused by rising levels of greenhouse gases, especially CO2 is a major global concern. In the future, our society will need to use CO2 and H2O to generate fuels for storage of renewable energy. Sequestration and fixation of atmospheric CO2 is central for limiting global warming and providing a non-petrochemical route to chemical building blocks such as CO, a key feedstock in large industrial processes. Therefore, it is essential to develop efficient catalysts for these reactions based on abundant and cheap metals. However, catalysts for CO2 conversion to CO still represent a major challenge for the field of chemistry. This in turn requires a fundamental understanding of how energy conversion processes happen in nature and of what it takes to make synthetic catalytic systems with performances and efficiencies as high as the biological ones. In this respect, understanding biocatalytic CO2 reduction offers enormous potential for guiding the design of novel catalysts needed for a sustainable circular energy economy to help close the CO2 cycle.Carbon monoxide dehydrogenases (CODHs) are nature’s catalysts for the CO2/CO interconversion, using earth-abundant metals in their active site. Ni-containing CODHs perform the two-electron reduction of CO2 to CO under physiological conditions with very high activity, selectivity and reversibility, relevant to the industrial electrochemical CO2 Reduction Reaction. They contain a unique [Ni–4Fe–4S] active site, and iron-sulfur clusters as electron relay.This project will focus on the biochemical characterisation of engineered CODH enzymes with novel properties and reactivities using recombinant and reconstitution methods to explore alternative metals. Mechanistic studies of the engineered CODH enzymes will be performed via an integrated approach combining electrochemical, spectroscopic, structural and computational methods.This is an interdisciplinary project encompassing biology, chemistry and biophysics disciplines. Novel methodologies and approaches will be developed to provide crucial insights into these fascinating enzymes, and to reveal design principles toward the development of artificial metalloenzymes for CO2 reduction. The supervisory team and associated members are early career researchers engaged in multidisciplinary and collaborative research, providing an excellent environment for the student to learn and develop crucial lab-based and interpersonal skills. |