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| **Scheme: GTA** |  |

School of Chemistry PhD Project Proposal Form

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| **Project Reference** | FastBioSpec |

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| **First Supervisor** | Dr Philip Ash |
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**Section 2 – *Project Information***

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| **Project Title** | Chemical energy conversion in biology studied using advanced spectroscopic and structural tools | |
| **Project Highlights:** | 1. | Understand natural chemical energy conversion through study of small molecule activation chemistry. |
| 2. | Work at large-scale national and international research facilities. |
| 3. | Gain a broad range of interdisciplinary skills that will open a wide range of future career paths. |
| **Project Description** | | |
| Redox properties of metal-containing active sites are critically important to many biocatalytic processes: one third of all proteins contain a redox-active metal, and ca 22% of submissions to the Protein Data Bank contain a transition metal. Metalloproteins capable of extracting energy from H2 gas, sequestering CO2 from the atmosphere, or performing complex monooxygenation reactions, rely upon the ability to access and control a range of often exotic metal oxidation states in an aqueous environment. Much of this crucial chemistry occurs at extremely fast rates, making it challenging to study using conventional structural and spectroscopic methods.  This project aims to investigate the catalytic mechanisms and structural dynamics of metalloenzymes that are vital for chemical energy conversion, with a focus on hydrogenase. State-of-the-art spectroscopic and structural studies will be combined with computational analysis to reveal critical but elusive transient intermediates by studying reactions in real time on sub-microsecond timescales. The outcomes of this project will provide a step change in our understanding of the mechanism of hydrogenase and other metalloenzymes, and will serve as inspirational catalysts for future green energy technologies  A PhD student will gain a broad range of interdisciplinary skills in spectroscopy, electrochemistry, chemical biology, structural biology, and biophysics whilst addressing critical questions about how nature achieves efficient chemical energy conversion. Together with the multidisciplinary research environment at the University of Leicester, this project provides an ideal means to gain crucial lab-based and interpersonal skills, as well as opportunities to undertake research at national and international research facilities.  **Techniques that will be undertaken during the project:**   * Computational modelling * Molecular Biology (cloning & mutagenesis) * Protein expression and purification * X-ray Spectroscopy * Time-resolved spectroscopy (infrared, Raman) * Synchrotron science * Chemical synthesis * Enzyme kinetics * Protein crystallisation * Structure determination | | |