Ph.D. Studentship

Development of *in situ* and *operando* neutron imaging for real-world reactor and reaction imaging

Heterogeneous catalysis plays a major role in many process operations adopted by the chemical manufacturing sector to produce a range of chemicals that are required by modern society. Recent initiatives by the University of Glasgow, the ISIS Neutron and Muon Facility and Johnson Matthey plc have exploited the capability of neutron scattering techniques to investigate a series of zeolite catalysed chemical transformations [1]. Johnson Matthey is a global-leader in sustainable technologies, with well-established interests in applied heterogeneous catalysis and reaction engineering.

Previous projects have employed the techniques of inelastic neutron scattering (INS) and quasi-elastic neutron scattering (QENS) to investigate zeolite catalysis, with the emphasis being on the development of a mechanistic understanding of the observed reaction chemistry [1]. However, there is an increasing awareness that the nature of the reactor also plays a contributory role, which can affect product distributions. Consequently, the GU/ISIS/JM team have recently used the technique of neutron imaging to further investigate a series of heterogeneously catalysed reactions. The IMAT neutron imaging operation at the ISIS Facility located at the Rutherford Appleton Laboratory (RAL) provides world-class capability, which can be employed to provide detailed images of how hydrogenous species are partitioned throughout a catalyst bed during reaction, enabling the implementation of *in-situ* and *operando* studies.

This new 4 year EPSRC Industrial CASE award project has two strands. The major programme of work is to use the technique of neutron imaging to investigate a series of hydrogenation reactions (*e.g.* selective alkyne hydrogenations) in a series of reactors. Initial measurements will concentrate on relatively straight-forward packed-bed tubular reactors, but these studies will be progressively extended to examine more specialised reactors such as the reactor technology used to produce sustainable aviation fuel [2]. The minor phase of the project will be to supplement the imaging measurements with complementary INS and QENS studies of the selected reaction systems. Thus, the project will provide experience in cutting edge catalytic science and reaction engineering that provides molecular insight over a range of length scales; from microscopic surface interactions to extended diffusion of gaseous reagents/products within bespoke and industrially relevant reactor configurations.

For the first year of study, the student will be based at the University of Glasgow, where the student will be instructed in the use of microreactors to test and evaluate certain catalyst formulations. Years 2 and 3 will be based at RAL, thereby ensuring good access to the world-class analytical facilities uniquely available at this location. Year 4 can be based at RAL or Glasgow. Each year, the student will be expected to spend a 1-2 week placement at Johnson Matthey's Technology Centre located in Berkshire.

The project is ideally suited to high-calibre graduates (≥ 2:1 degree) in Chemistry, Chemical Engineering, Chemistry and Medicinal Chemistry and/or Chemical Physics, providing a rigorous training in surface chemistry and heterogeneous catalysis research. A tax-free stipend of *ca*. £18,622 *p.a*. for 4 years is provided alongside the payment of all University fees. *Eligibility is restricted to UK citizens only.*

References

[1] A. Zachariou et al., *Catal. Sci. Technol.*, 13 (2023) 1976; **[2]** M. Peacock et al., *Top. Catal.*, 63 (2020) 328.

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