Imperial College London

Chemical Transport and Adsorption in Hierarchical Porous Solids

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Funding and Deadline: To be eligible for support, applicants must be "UK Residents" as defined by the EPSRC[1]. The studentship is for 3.5 years starting in October 2022 and will provide full coverage of standard tuition fees and an annual tax-free stipend of approximately £17,609. Applicants should hold or expect to obtain a First-Class Honours or a high 2:1 degree at Master's level (or equivalent) in Chemical Engineering, another branch of engineering or a related science. Funding is through the project InFUSE (Interface with the future: underpinning science to support the energy transition), funded by the EPSRC and Shell.

Project summary

The rational design of porous solids that perform under reaction conditions remains a very attractive prospect in materials research. In gas separations applications, the continued search for novel formulations with improved separation factors aims at enabling transformative step changes beyond classic adsorbents. The processing of the adsorbent into its macroscopic technical form (*e.g.*, pellets, monoliths) is a critical element in this endeavour and offers opportunities for radical innovations. These shaped adsorbent formulations feature spatial variations in chemical composition and include multimodal porous structures made of interconnected pores with vastly different sizes. Elucidating the equilibrium and kinetic adsorption parameters of these systems remains therefore very difficult. One experimental challenge is in probing the concentrations of both gas and adsorbed species at the required spatial and temporal resolution, requiring approaches where complementary data are acquired (*e.g.,* imaging with diffraction) concurrently.

The project aims to develop and test an experimental workflow to characterise gas transport in microporous solids and correlate it to changes in the solid framework resulting from gas adsorption. Recent achievements in synchrotron-based experimentation provide unprecedented opportunities in this area – enabling the quasi-simultaneous acquisition of x-ray tomograms (for imaging) and diffraction patterns on the microscale within the same sample at the same location. The Diamond Light Source – the UKs national synchrotron facility – is a key partner in the project and will support the design of novel environments to study samples under *operando* conditions. We will consider both classic and novel adsorbent formulations. The obtained imagery will be used alongside numerical tools to link pore-scale observations to the continuum scale. The ability to monitor the functioning of technical porous solids by means of *operando* synchrotron experiments will enable creating a direct link between material structure and performance, disclosing new opportunities for the rational design of the materials themselves. The core application considered here is gas separations, but these developments will apply to other processes utilising hierarchical porous solids, such reactive transport in rocks or battery electrodes.

Informal enquiries about the post and the application process can be made to Dr Ronny Pini by including a motivation letter and CV.

Eligibility for student funding: https://www.ukri.org/councils/esrc/career-and-skills-development/funding-for-postgraduate-training/eligibility-for-studentship-funding/