Metal-organic frameworks (MOFs) have been of interests to the scientific community due to their great tunability in porous structures and chemical properties for various applications such as gas adsorption and storage. Cu₃(BTC)₂ framework (copper benzene-1,3,5-tricarboxylate or HKUST-1), is a well-studied MOF
for gas separation and storage. To date, CO$_2$ adsorption on HKUST-1 is primarily focusing on manipulating the CO$_2$ adsorption capacity/selectivity by using materials design strategies or post-synthetic modification approaches. In this work, we focused on using dynamic water vapour adsorption experiments to investigate the hydration process of HKUST-1 framework under various humid conditions and assess its moisture stability. Results obtained lead to (i) the underlying mechanism of HKUST-1 MOF decomposition upon the exposure to humid flows and (ii) strategies of designing new MOFs (based on HKUST-1) or new processes for employing original HKUST-1.

This talk will show our Grand Canonical Monte Carlo (GCMC) simulation work on investigating the effect of structural defects (pore blockages and structural defects) in HKUST-1 MOF on pure CO$_2$ adsorption forming a quantifiable approach that can quickly identify key defective features of the porous structure of HKUST-1 that influence its adsorption performance.

Abstract

Xiaolei received his BEng (Environmental Engineering) and MRes (Chemical Engineering) in China. In 2006, he joined the Department of Chemical Engineering at the University of Bath, UK, as a PhD candidate under the supervision of Prof. Alexei A. Lapkin. His PhD projects focused on designing structured multifunctional reactors, formulating novel carbon-based metal catalysts for continuous-flow heterogeneous catalysis and developing flow chemistry with microreactors. After his PhD, from May 2010 to September 2013, Xiaolei worked as a post-doctoral research fellow at the University of Warwick and then at the University of Cambridge. During this period, He was contracted by EC FP7 projects to develop nanomaterial-based catalysts (e.g. bi-metallic catalysts supported on monoliths coated with nanocarbons) and perform multi-scale modeling (CFD + kinetic modeling) of catalytic multiphase flows in structured reactors.

In October 2013, he joined the School of Chemical Engineering and Analytical Science (CEAS) at The University of Manchester as a Lecturer in Chemical Engineering. He has a research group with 6 PhD students and one PDRA with research projects focusing on (i) engineering microporous materials (MOFs) for carbon dioxide capture, (ii) hierarchical catalytic structures based on open-cell SiC foams for water treatment, (iii) bimetallic nano-structures for catalytic upgrading of bio-oils, (iv) mechanistic kinetic modelling of catalytic reactions and (v) novel catalysts based on MOFs and polymers.

Date: 6 October 2015 (Tue)
Time: 2:00pm
Venue: Room 1504 (Lift 25/26)