NECEM SEMINAR: "Computational discovery of molecular materials"
Dr Kim Jelfs, Imperial College, London

15:00pm-16:00pm, Wednesday 26th June 2019

Lecture Theatre 1.75, Bedson Building, Newcastle University

Refreshments available after the seminar

Computational discovery of molecular materials

We have been developing computational software towards assisting in the discovery of molecular materials with targeted structures and properties. Whilst initially we have focused upon porous molecular materials, we will also address the ways in which our approach is generalisable to other molecular materials and their applications, including as organic semiconductors or for photocatalysis. Intrinsically porous organic molecules have shown promise in separations, catalysis, encapsulation, sensing, and as porous liquids. These molecules are typically synthesised from organic precursors through dynamic covalent chemistry (DCC). If we consider cages synthesised from imine condensation reactions alone, there are approximately 800,000 possible aldehyde and amine precursors, combining these in all the different possible topologies results in over 830 million possible porous organic cages. Therefore, either from a computational or synthetic perspective, it is not possible for us to screen all these possible assemblies. Our evolutionary algorithm automates the assembly of hypothetical molecules from a library of precursors. The software belongs to the class of approaches inspired by Darwin's theory of evolution and the premise of "survival of the fittest". Our approach has already suggested promising targets that have been synthetically realised. Further, we are addressing questions such as which topologies or DCC reactions maximise void size or whether specific chemical functionalities promote targeted applications. We have also examined the application of machine learning for the rapid prediction of whether porous organic molecules will be shape persistent, retaining an internal cavity, or not.

Biography

Dr. Kim Jelfs is a Senior Lecturer and Royal Society University Research Fellow (URF) in the Department of Chemistry at Imperial College London, UK. Her group specialises in the use of computer simulations to assist in the discovery of supramolecular materials. This includes the development of software to automate the assembly and testing of materials, with the application of artificial intelligence techniques including an evolutionary algorithm. The materials studied include porous materials for molecular separations or materials for the generation of renewable energy.

Kim completed her PhD in Computational Chemistry at UCL (UK) in 2010, studying the crystal growth of zeolitic materials. She worked as a post-doctoral researcher conducting simulations across the experimental groups at the University of Liverpool, before beginning her independent research at Imperial College in 2013. She was awarded a 2018 Royal Society of Chemistry Harrison-Meldola Memorial Prize and holds an ERC Starting Grant.

Location
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