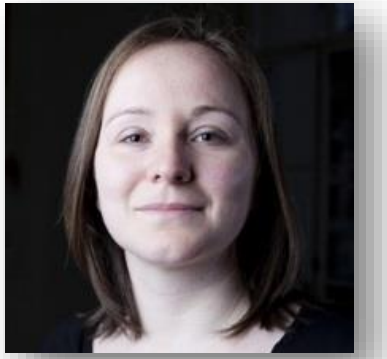
Warwick Chemistry Departmental Seminar



Dr Kim Jelfs

Imperial College London

Thursday 14 February

4.00 pm, Physics Lecture Theatre, Science Concourse

‘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

Kim Jelfs is a Senior Lecturer and Royal Society University Research Fellow and specialises in the use of computer simulations to assist in the discovery of supramolecular materials. After a PhD modelling the crystal growth of zeolites at UCL, she worked as a post-doc across the experimental groups at the University of Liverpool, before beginning her independent research at Imperial College in 2013. She was awarded a Royal Society of Chemistry Harrison-Meldola Memorial Prize in 2018.