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Introduction to Synthesis 4.0: towards an internet of chemistry

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Across the industrial landscape, interconnected technology is igniting a fourth industrial revolution (Industry 4.0), one that unifies machines, devices, automation, and artificial intelligence to deliver smart manufacturing solutions to global challenges. Just as the Internet of Things has transformed manufacturing, an Internet of Chemistry is emerging that will shape how cyber-technologies are used in chemical research. Highlighted in this themed issue, the arrival of the "Synthesis 4.0" trend is enabling experimentation to be performed more efficiently and rapidly, generating richer sets of data that invite a multidisciplinary approach to synthesis and process optimization.

In the UK, the Dial-a-Molecule Grand Challenge Network (http://generic.wordpress.soton.ac.uk/dial-a-molecule/)

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Dr Richard A. Bourne

Richard Bourne completed a PhD under the supervision of Prof. Martyn Poliakoff, CBE, FRS at the University of Nottingham. He is now working as an Associate Professor at the University of Leeds on the development of new sustainable processes with focus on automated continuous flow routes to pharmaceutical and fine chemical products. His group is based within the Institute of Process Research and Development (IPRD) a joint institute between Chemical Engineering and Chemistry. Richard is particularly interested in the use of automated flow systems combining online analysis, feedback control and evolutionary algorithms to provide process understanding and optimisation. This particularly interdisciplinary research at the interface between Chemistry and Chemical Engineering aims to develop processes at laboratory, pilot plant and manufacturing scales. Richard has developed several industrial platforms and held a Royal Academy of Engineering Industrial Fellowship in 2015 at AstraZeneca Macclesfield, which in 2018 led to the EPSRC project "Cognitive Chemical Manufacturing" developing integration of machine learning approaches to chemical processes.

King Kuok (Mimi) Hii

Mimi Hii obtained her BSc(Hons) and PhD degrees from the University of Leeds, before pursuing postdoctoral research work at Oxford University with Dr John M. Brown, FRS. Her independent academic career began with an award of a Ramsay Memorial Fellowship, and a lectureship appointment at King's College London. In 2003, she moved to Imperial College, and was promoted to a Professorship in 2016. She was elected as a Fellow of the Royal Society of Chemistry (FRSC) in 2013. In 2019, she was appointed as an Associate Editor for ACS Sustainable Chemistry & Engineering.Over the course of her career, Mimi assembled an extensive programme of research into catalytic reactions and processes. In the last decade or so, she has collaborated widely with colleagues in Chemical Engineering in advancing novel reaction technologies to multiphasic (catalytic) reactions. In 2018, she led a successful bid to establish the UK's first Dial-a-Molecule Grand Challenge Institute: the Centre for Rapid Online Analysis of Reactions (ROAR). In the same year, she also secured funding to establish the EPSRC Centre for Doctoral Training in Next Generation Synthesis & Reaction Technology, to provide training in data-led chemistry.

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was formed in 2010 to provide a forum for transforming the way in which synthetic chemistry is carried out, moving away from slow, labour-intensive manual methods, to highly automated, data-driven approaches. For these ideals to be realised, synthetic chemistry research needs to continue evolving by embracing advances in data science and automation, such as to accelerate the discovery process that is necessary to address increasing global demand for better agrochemicals, smart materials, and medicines.

Indeed, the way synthesis is practised has changed substantially over the past decade: the use of high-throughput automated equipment is now routinely used to execute a large number of reactions in parallel, for screening multiple reaction parameters rapidly, such as reactant-catalyst-solvent combinations (*e.g.* DOI: 10.1039/C9RE00054B, 10.1039/C9RE00067D, 10.1039/C9RE00118B), where multivariate analysis (MVA), statistical, or mechanistic methods can be applied to large datasets to extract reaction understanding (DOI: 10.1039/C9RE00072K, 10.1039/C9RE00180H, 10.1039/C9RE00086K). The use of smart devices and technologies (*e.g.* data visualisation, networked systems, online analytics, robotics, and internet connected devices) is becoming increasingly prevalent in chemical laboratories (DOI: 10.1039/C9RE00017H, 10.1039/C9RE00057G, 10.1039/C9RE00144A, 10.1039/C9RE00043G). Greater accessibility of these devices to the scientific community has led to the emergence of all-in-one reaction characterization and optimization platforms. These platforms merge automated equipment with online analytical tools and algorithms, again in an effort to deliver richer process data and better understanding (DOI: 10.1039/C9RE00116F, 10.1039/C9RE00072K, 10.1039/C9RE00078J, 10.1039/C8RE00345A, 10.1039/C9RE00087A, 10.1039/C9RE00096H). In the digital space, algorithms continue to be refined for application of rule-based and machine learning methods to the prediction of synthetic routes (10.1039/C9RE00076C, 10.1039/C9RE00019D).

By assembling this themed issue, the editors would like to highlight the unique opportunities and challenges of adopting a data-driven approach to synthesis. Working with multidisciplinary contributors across disciplines and from academia and industrial laboratories, we are pleased to present a collection of articles across the theme of "Synthesis 4.0" to highlight state-of-the-art research as well as future challenges. Last but not least, we would like to thank all the contributors for their submissions to this themed issue, which we hope will help to encourage the future expansion of this impactful research area.

Brandon J. Reizman

Brandon Reizman is an associate senior consultant engineer in Small Molecule Design and Development at Eli Lilly and Company. He has a B.S. in chemical engineering from the University of Illinois at Urbana-Champaign and both an M.S. and a Ph.D. in chemical engineering from the Massachusetts Institute of Technology. At MIT, his thesis research focused on the design and application of kinetic modeling tools for the purpose of conducting automated, self-optimizing chemical experiments. In 2015, he joined Eli Lilly as a process development engineer, where he has supported initiatives in continuous manufacturing and in the increased usage of predictive modeling strategies in pharmaceutical development. He was recognized as one of Lilly Research Laboratories' top 100 innovators in 2018.