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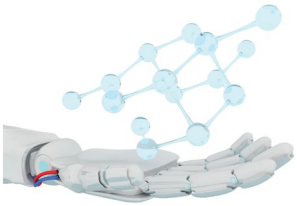
Automate and digitize

In this issue, we focus on the combination of techniques such as machine learning, artificial intelligence, robotics and automation for the synthesis of chemicals and materials.



Automating synthesis accelerates research and development and now, with the increase in prevalence of machine learning (ML) and artificial intelligence (AI) techniques, research is being accelerated to a greater degree than ever before[1–4]. In this issue of *Nature Synthesis*, we present a range of articles which showcase developments in the automation and digitalization of chemistry and materials synthesis, as well as highlight some of the key challenges to be overcome so that these technologies may continue to improve and be more widely used by researchers.

In a Review featured on the cover of this issue by Milad Abolhasani and Eugenia Kumacheva, the development of self-driving laboratories is outlined and a roadmap for the implementation of self-driving laboratories is provided. The current limitations of this technology, such as the lack of standardization of hardware modules, data flow, data representation and experiment-selection algorithms are discussed. Furthermore, interesting future developments in this area, such as remote operation capabilities through the cloud or remote connection, are highlighted.

A Review by John Gregoire, Lan Zhou and Joel Haber describes the use of combinatorial synthesis with AI for the acceleration of materials science. Ten metrics for evaluating a combinatorial synthesis technique for use in a given experimental workflow are proposed, covering speed, scalability and scope, for example. From this evaluation, opportunities for development of various combinatorial synthesis techniques are elucidated, such as automated decision-making using AI.

In a Comment by Jonghee Yang and Mahshid Ahmadi, the use of data-driven automated experimentation in materials synthesis is discussed, including how ML algorithms integrated into experimental workflows interpret datasets generated from automated experiments, allowing latencies to be identified and new experimental conditions to be proposed. Additionally, challenges in using ML algorithms to predict optimal experimental conditions based on chemical and physical models are highlighted.

In a Comment by Junliang Liu and Jason Hein, the combination of automated data-gathering techniques with ML and AI tools is described for accelerating reaction discovery. We learn about the use of real-time reaction monitoring to provide comprehensive data, such as reaction kinetics and by-product reaction pathways, as well as how this data can be used to train predictive models.

A Q&A with Mimi Hii reveals key hardware and software challenges to be overcome in automated synthesis. Additionally, we learn about the Centre for Rapid Online Analysis of Reactions, which aims to provide researchers with access to automation equipment, as well as advice, training and support on the use of this equipment, thereby educating a new generation of chemical scientists and engineers who can work seamlessly between chemistry, engineering and data science fields.

In a Q&A with Andrew Cooper, the use of robotics and AI for the synthesis of materials and chemicals is discussed. We learn about the challenges in designing robotic systems to perform experiments with low failure rates, and how AI may be used to prevent or recover from errors in the future. Furthermore, the Materials Innovation Factory is discussed, which aims to allow researchers in academia and industry to utilize automation, computation and digital methods for the discovery of new materials.

In an Article by Zhao et al., a robotic platform is developed for the synthesis of gold and double perovskite nanocrystals. Data mining of the literature is used to obtain initial synthetic parameters which are used for the automated synthesis and in situ characterization. Additionally, ML models identify correlations between the morphologies of the products and structure-directing agents, thereby improving the platform over time as the ML models are trained on the continuously expanding experimental dataset.

An Article by Wu et al. demonstrates a high-throughput approach for the exploration of functional polypeptide chemical space by diversifying polypeptides through reactions between selenolate and a variety of electrophiles. Automation of this approach allows 1,200 homopolypeptides or random heteropolypeptides (RHPs) to be prepared in one day, and ML is employed to explore the RHP library for polypeptides with improved glutathione peroxidase-like activity. A News & Views article by Adam Gormley describes how approaches for preparing polymers with protein-like behaviour in this way are likely to play a key role in preparing synthetic mimics of biological structures in the future.

Additionally, a Research Highlight based on work by Abigail Doyle and co-workers describes a statistical modelling approach to learn about interaction effects in high-throughput experimentation datasets. And in a Research Highlight based on work by Connor Taylor, Alexei Lapkin and co-workers, we learn about the use of multi-task Bayesian optimization to accelerate the optimization of pharmaceutically relevant reactions when combined with a self-optimizing flow reactor.

The increase in usage of automation and data in synthesis provides an exciting glimpse into the future of chemicals and materials preparation, which shows no signs of slowing down. For example, the University of Toronto's Acceleration Consortium has recently been awarded $200 million to support self-driving laboratory research, highlighting the great interest in this field for the future. From self-driving labs to the use of advanced algorithms for reaction prediction, we are seeing many interesting technologies that hold great promise to accelerate research and development, and we look forward to seeing what advancements come next.

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