

Key role of AI in delivery of sustainable chemical solutions

Alexei Lapkin

Department of Chemical Engineering and Biotechnology, University of Cambridge, UK
aal35@cam.ac.uk

While the target of most discovery/development projects is on the main function of a molecule (therapeutic action, performance as part of a consumer product, etc), the cost of delivery of the main function, especially extended to life cycle and social impacts is becoming a key element of the design vector. Debates about 'what is sustainable' are still ongoing, while industry has focused on a small number of sustainability targets, such as reduction in the climate change-linked emissions. Even this single target has significant implications across the complete value chain of chemistry, as this affects the choice of feedstocks, solvents, reagents, locations for manufacture, preferred technologies, delivery modes and business models. AI tools are critical in supporting the decision making in design and development of new molecules. From molecular design for main function to the multi-criteria design over the expanded design vector that includes sustainability targets, AI tools enable to navigate highly non-linear multi-parameter space to identify globally optimal solutions.

In this talk I will specifically address the issue of clean synthesis. I will discuss the incorporation of fossil-free starting materials and reagents into synthesis planning, the inclusion of sustainability metrics into synthesis plans and how computer aided synthesis planning helps in identification of more elegant and cleaner solutions.