

## **Integrating process and molecular design: a journey across scales**

The performance of chemical processes depends not only on flowsheet structure, equipment design and operating conditions, but also on the choice of processing materials such as catalysts and solvents. Using a different solvent, for instance, can change the rate of a reaction by several orders of magnitude. Despite this, processing materials are often selected very early process development, leading to sub-optimal process performance.

In this seminar, we explore how better designs can be developed by integrating molecular and process design decisions. Given the number of potential solutions to this extended design problem, and the complexity of the task, computer-aided design techniques and multiscale models have an important role to play in identifying promising options, thereby providing focus for experimental studies. We highlight the key challenges that must be overcome to enable such multiscale design and demonstrate what can be achieved on different processes.