Wolfson Department of Chemical Engineering Seminar

Monday, December 29, 2025 at 13:30–14:30

Room 6

From First Principles to Decision-Grade Kinetics: Toward Autonomous Chemical Discovery

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Predictive chemical kinetic modeling aims to determine how reactive systems evolve from given initial conditions with enough fidelity to guide design and optimization in Chemical Engineering. In this talk, I will outline my group's contributions to making this promise operational, through three threads: basic science, engineering applications, and closed-loop autonomous discovery.

First, we will walk through the basic tools our group develops and uses, primarily the Reaction Mechanism Generator (RMG) software and the Automated Rate Calculator (ARC) tool, which can together generate a chemical kinetic model and refine it using ab initio methods. Then we will see some of the applications we worked on, emphasizing prior misconceptions in the literature, along with our "from first principles" philosophy. As time permits, we will cover two computational studies outside the chemical kinetics field: automated generation of novel energetic materials and predicting the hard protein corona sphere that forms on nanoparticles. Two examples for basic science research will be discussed, specifically mapping atoms in a reaction considering 3D effects, and automatically searching for reaction transition states.

Finally, we will close with a preview of our next leap: a closed-loop, agentic AI platform that couples predictive chemical kinetic modeling with a self-driving PFR. The goal is decision-grade, generalizable kinetics: reliable enough to design with, and automated enough to scale.

(Refreshments will be served at 13:15)