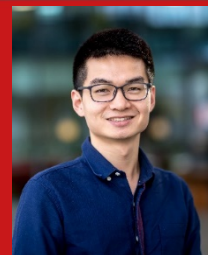


# Computer-assisted continuous-flow photochemistry

Zhenghui Wen & Timothy Noël

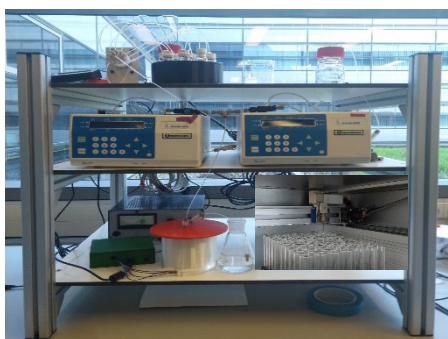


## Introduction

Continuous-flow photochemistry receives a lot of attention from researchers as this technology provides reduced reaction times, higher selectivity, and safe operation. However, the discovery of chemical reactions is an inherently unpredictable and time-consuming process. An attractive alternative is to predict reactivity, although relevant methods, such as computer-assisted reaction design, are still in their infancy. Inspired by this strategy, we propose that a reaction system controlled by computer algorithm may be able to explore the space of chemical reaction quickly.

## Project summary

Currently two topics are being studied: a fully automated platform for continuous-flow photochemistry and photochemical synthesis are in development.



In order to accelerate the screening of the continuous-flow photoreaction and development of new photocatalytic reactions, a fully automated platform, containing reagent storage, selection, pumping, mixing, reaction, analysis and sample collection, is being established. This platform is still in the development phase and some control codes need to be programmed and optimized.

For the purpose of assessing the applicability of this automated platform, several photochemical reaction are under consideration. The reaction with easy operation, mild reaction condition and high-value product are highly recommended. And then, more complicated reaction can be investigated.

## Project goals

Typical MSc projects contain the development of automated platforms, reaction optimization and recognition of spectrum. BSc projects typically contain reaction optimization and program optimization.

Generally, reactions are performed in liquid phase, mainly about the trifluoromethoxylation.

## Contact information

Zhenghui Wen: z.wen1@tue.nl, STO 1.40.

Timothy Noël: t.noel@tue.nl, STO 1.37.

CHEMICAL ENGINEERING AND CHEMISTRY

