

Digital Chemistry for Applied Catalysis – a Discussion

28 November 2023, Burlington House (RSC), Piccadilly, London, W1J 0BA, UK

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Introduction

A one-day discussion style meeting at Burlington House providing an opportunity to discuss the impact of digital chemistry techniques on the field of Applied Catalysis. As well as oral contributions from leading practitioners in academia and industry in the field, there will be a poster session and opportunities to discuss what opportunities digital techniques will provide as the field moves forward and network with others interested in this exciting field.

Invited Speakers:

Understanding reactivity trends in Ni-Suzuki reaction

Megha Anand (Astra Zeneca)

Understanding applied catalysis through modern atomistic modelling

Andy Logsdail (Cardiff University)

Decisions from Data – Predictions for Organometallic Catalysis

Natalie Fey (Bristol University)

Exploring ligand space with CSD, DFT calculations and AI/Machine Learning

Bao Nguyen (Leeds University)

Industrial IOT in the Process Sector: a Case Study

Carl Tipton (Johnson Matthey)

Biocatalysis and Enzyme Engineering in the Digital Era

Joseph Hosford (GSK)

Advancements in Machine Learning Approaches for Large-Scale Chemical Imaging Data Processing

Hongyang Dong (UCL/Finden Ltd.)

Programme

The event will include perspective talks from a mix of industrial and academic invited speakers, as well as the opportunity to network and for students/younger members to present posters:

Poster setup available	09:30 – 10:00
Registration coffee and posters	10:00 – 10:45
Talks	10:45 – 12:45
Discussion/Panel 1	12:45 – 13:15
Lunch	13:15 – 14:05
Talks	14:05 – 15:25
Break	15:25 – 15:55
Talk	15:55 – 16:35
Discussion/Panel 2	16:35 – 17:05
Talk	17:05 – 17:45
Drinks reception	17:45 – 18:30

Registration and Website

<https://www.rsc.org/events/detail/76908/digital-chemistry-for-applied-catalysis>

Please see the website for details on registration and poster abstract submission.

	Standard
RSC member registration fee	£140
Non-member registration fee	£155
Student RSC member registration fee	£60
Student non-member registration fee	£80

Bursaries

We are pleased to offer a limited number of free registrations to students who are accepted to present a poster where this would enable them to attend – please contact the organizers using the contact form on the website (first-come, first-served).

Exhibition Opportunities and Sponsorship

We rely on the generosity of our sponsors in order to keep registration costs as low as possible! There will also be a small exhibition of relevant trade stands. Please contact us using the contact form on the above weblink under the “contact” section for details of further sponsorship / exhibition opportunities.

About the ACG

This event is organized by the RSC Applied Catalysis Group (ACG). The Applied Catalysis Group aims to promote both hetero- and homo-generous catalysis through a range of activities including seminars, conferences and other professional activities related to chemical catalysis.

Organizing Committee

Simon Beaumont (*Durham University*); Paul Collier (*Johnson Matthey*); Gregory Price (*RSC Applied Catalysis Interest Group*); Katherine Wheelhouse (*GSK, UK*); Keith Whiston (*RSC Applied Catalysis Interest Group Chairman*).