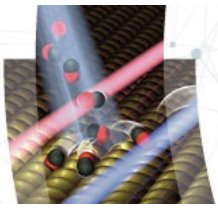
Bridging the gap from surface science to heterogeneous catalysis

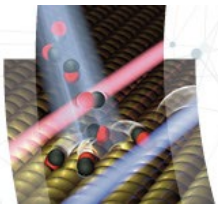
20–22 April 2026 | London, UK



Faraday Discussions

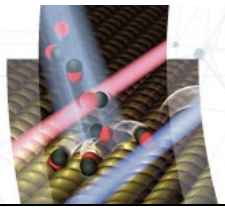
Day 1

11:00	Registration and refreshments
12:00	Lunch
12:45	**Welcome and introductions** Alec Wodtke and Matthias Scheffler, *Co-chairs of Scientific Committee*
12:55	**Outline of Discussion format** Donna Smith and Kevin Vincent, *Royal Society of Chemistry Publishing Editors*
13:00	**Introductory Lecture – Spiers Memorial Lecture** (Session chair:) Jens Norskov *Technical University of Denmark, Denmark*
	Session 1: Chemical mechanisms and system analysis in heterogeneous catalysis (Session chair:)
14:00	**Microcalorimetric Quantification of Hydrogen Adsorption Thermodynamics in Water-Solvated Systems on Pt/C** David Flaherty *Georgia Technical University, USA*
14:05	**What can Raman spectroscopy really say about the adsorbed CO on roughened Cu electrodes in CO_2 electroreduction conditions?** Anastassia Alexandrova *UCLA, USA*
14:10	**Disentangling multistep kinetics by combining electrochemical Arrhenius analysis with micro-kinetic modelling** Mathieu Lizée *Fritz-Haber Institut of the Max Planck Society, Germany*
14:15	Discussion
15:30	Refreshments
16:00	**Critical Assessment of Theoretical Modelling of Single-Atom Catalysts** Gianfranco Pacchioni *Università Milano-Bicocca, Italy*
16:05	**Compensation effects between the apparent activation energy and pre-exponential factor in simple models of electrocatalytic hydrogen evolution** Marc Koper *Leiden University, Netherlands*
16:10	**Thermophysical properties of adsorbates with beyond-DFT accuracy from DFT data through error cancellation** Bjarne Kreitz *Georgia Institute of Technology, USA*
16:15	Discussion
17:30	Lightning presentations (by invitation of the Scientific Committee)
18:00	Poster session and wine reception
19:30	Close

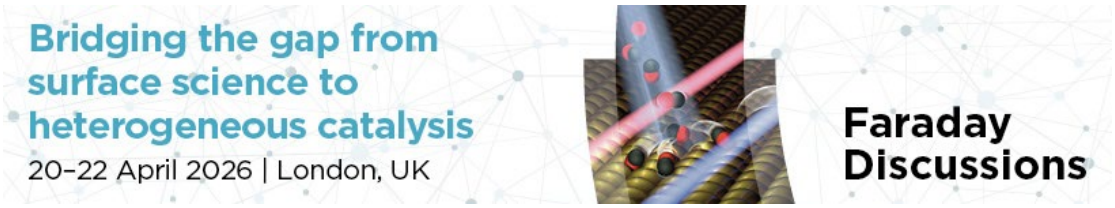


Day 2

	Session 1 (cont.): Chemical mechanisms and system analysis in heterogeneous catalysis (Session chair:)
09:00	**Competing reaction pathways in decomposition of 2-propanol over V-doped Co_3O_4(111) model catalyst: a mechanistic study** Swetlana Schauermann *Kiel University, Germany*
09:05	**The effect of adsorbate induced surface strain on oxygen island formation on platinum surfaces** Florian Nitz *Georg-August University of Göttingen, Germany*
09:10	**CO on a Rh/Fe_3O_4 single-atom catalyst: high-resolution infrared spectroscopy and near-ambient-pressure scanning tunnelling microscopy** Gareth Parkinson *TU Wien, Austria*
09:15	Discussion
10:30	Refreshments
	Session 2: Impact of Artificial Intelligence on Heterogeneous Catalysis (Session chair:)
11:00	**Rethinking Catalysis: Interpretable AI and Description of Real-World Conditions via Materials Genes** Lucas Foppa *Fritz Haber Institute of the Max Planck Society and MS1P e.V., Germany*
11:05	**Size-dependent kinetic restructuring of catalyst active sites: A MACE-APE study of fluxional Pdn/MgO (n=3-11) clusters** Patricia Poths *Fritz Haber Institute of the Max Planck Society, Germany*
11:10	**Interpretable Bayesian Optimization for Catalyst Discovery** Akhil S. Nair *Fritz-Haber Institute of the Max-Planck Society, Freie University Berlin, Germany*
11:15	**Carbon Dioxide Hydrogenation on Copper and Nickel Catalysts via a Conformal Sampling Approach** Alessandro Fortunelli *CNR, Italy*
11:20	Discussion
13:00	Lunch
	Session 2 (cont): Impact of Artificial Intelligence on Heterogeneous Catalysis (Session chair:)
14:00	**A consistent dynamics view on nanoporous catalysts in action across length and time scales** Veronique Van Speybroeck *Ghent University, Belgium*
14:05	**Role of monodentate formate in product selectivity for CO_2 hydrogenation on Pd-based alloy catalysts** Igor Kowalec *Cardiff University, UK*
14:10	**An Interpretable Machine Learning Framework for Prediction of Adsorption Energies and Generative Design of Active Sites on Arbitrary Catalysts** Matthew Johnson *Sandia National Laboratories, USA*
14:15	Discussion
15:30	Refreshments
	Session 3: New experimental methods for observing catalysts in action (Session chair:)



16:00	**TBC** Stig Helveg *Technical University of Denmark, Denmark*
16:05	**Surface orientation-dependent electro-oxidation of a polycrystalline gold electrode** Edvin Lundgren *Lund University, Sweden*
16:10	**Structure-Controlled Sulfur Poisoning and Hydrogen-Induced Regeneration in Single Pd Nanoparticles Probed by Nanospectroscopy** Elad Gross *The Hebrew University of Jerusalem, Israel*
16:15	Discussion
17:30	Close of sessions
18:30	Pre-dinner drinks
19:00	Conference dinner



Day 3

	Session 3 (cont.): New experimental methods for observing catalysts in action (Session chair:)
09:00	**The Ever-Evolving Active Site: Transformation of Single Atoms to Extended Structures during Rh-catalyzed Reverse Water-Gas Shift Reaction** Simon Bare *SLAC, USA*
09:05	**Operando XPS Studies of precisely size-selected Pd nano-catalysts for methane oxidation** Georg Held *Diamond Light Source, UK*
09:10	**Monitoring Ammonia Oxidation on Pt(332) at non-stationary Oxygen Coverages: Convergence of Microkinetic Simulations and Experiment** Stefan Hörandl *Georg August University Goettingen, Germany*
09:15	Discussion
10:30	Refreshments
	Session 4: Rational Design of Dynamic and Self-repairing Active Sites (Session chair:)
11:00	**Evolution of Size-Selected Pt Cluster Catalysts on Prototypical Oxide Supports** Barbara Lechner *TU Munich, Germany*
11:05	**Developing the Science of Self-Healing Catalysts** Abhaya Datye *University of New Mexico, USA*
11:10	**Ionic Liquid Overlayers Stabilize Ligand-coordinated Oxide-supported Single-atom Pd Heterogeneous Catalysts for Partial Hydrogenation of Acetylene** Steven Tait *Indiana University, USA*
11:15	**Correlating binding energies of adsorbed CO and H on model surfaces with CO/H_2 selectivity from co-electrolysis of CO_2 and H_2O over copper-palladium bimetallic catalysts** Jingguang Chen *Columbia University, USA*
11:20	Discussion
13:00	**Concluding Remarks Lecture** (Session chair:) **Faraday Discussion on Surface Science and Heterogeneous Catalysis, A View From The Bridge** Simon Beaumont *Durham University, UK*
13:30	**Acknowledgements**
13:45	**Close of meeting and lunch**

Presenting authors are indicated in the programme by an underline. The affiliation is for the presenting author. If the presenting author of your paper has changed since abstract selection please email events@rsc.org. Please note that this is a draft programme and timings may change.