Pre-conference session (online-only)

Aimed particularly at early career researchers but open to everyone, our online-only programme on Friday features opportunities for networking and discussion before the start of the conference proper.

Friday 24 March 2023 (timings are GMT)

Join our online discussion rooms for a chance to discuss the papers with your peers ahead of time. Facilitated by a member of the scientific organising committee and hosted on the conference platform, these online discussion rooms will be informal in nature and do not form part of the official discussion. There will be five rooms, each dedicated to one of the sessions in the programme. Sessions will run simultaneously, and you are free to drop in or out as you wish. Attendance is included in your registration – take part by simply clicking on your unique joining link.

13:00 – 14:30	**Early career discussion rooms** • Heterogeneous catalytic and chemical looping routes to N2 activation • Enzymatic N2 activation • Electrocatalytic and photocatalytic routes to N2 activation • Homogeneous N2 activation • Alternative routes to NH3 and its application

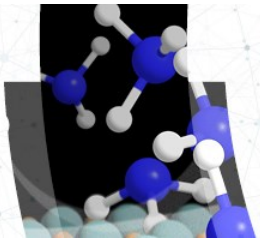
The discussion room session will be followed by a dedicated online poster session -- an opportunity for delegates attending online to present their work and discuss it with other delegates. In-person poster presenters are welcome to upload a digital version of their poster and present it in this session if they wish.

14:30 – 15:30	**Online poster session**

Please note that the UK time zone changes from GMT to BST on Sunday 26 March.

Sustainable nitrogen activation

27-29 March 2023 | London, UK and online



Faraday Discussions

Monday 27 March 2023 (timings are BST)

12:00	Registration and lunch
12:45	**Welcome and introductions** Justin Hargreaves *Chair of Scientific Committee* *University of Glasgow*
12:55	**Outline of Discussion format** *Royal Society of Chemistry Publishing Editors*
13:00	**Introductory lecture** (Session chairs: Richard Catlow and Kylie Vincent) Hideo Hosono *Tokyo Institute of Technology, Japan*
	Session 1: Heterogeneous catalytic and chemical looping routes to N2 activation (Session chair: Justin Hargreaves and Ping Chen)
14:00	**Barium hydride activates Ni catalyst for ammonia synthesis** Wenbo Gao* *University of Chinese Academy of Sciences, China*
14:05	**Ionic conductivity and disorder in calcium and barium nitrogen hydrogen phases** Gavin John Irvine *University of St Andrews, UK*
14:10	**The formation of lithium-iridium complex hydride toward ammonia synthesis** Qianru Wang* *Chinese Academy of Sciences, China*
14:15	Discussion
15:30	Refreshments
	(Session chair: Ping Chen and Justin Hargreaves)
16:00	**Structural evolution of TiN catalysts during mechanocatalytic ammonia synthesis** Carsten Sievers *Georgia Institute of Technology, USA*
16:05	**Mechanism of ammonia synthesis on Fe3Mo3N** Michael Higham *University College London, UK*
16:10	**Experimental and theoretical investigations on the anti-perovskite nitrides Co3CuN, Ni3CuN and Co3MoN for ammonia synthesis** Angela Daisley *University of Glasgow, UK*
16:15	**Switching on/off molybdenum nitride catalytic activity in ammonia synthesis through modulating metal support interaction** Jean-Philippe Dacquin *Université de Lille, CNRS, France*
16:20	Discussion
18:00	Flash poster presentations (by invitation of the scientific committee)
18:30	Poster session and wine reception
20:00	Close of sessions

Tuesday 28 March 2023 (timings are BST)

	Session 1 (cont.): Heterogeneous catalytic and chemical looping routes to N2 activation (Session chair: Richard Catlow and Andrew Hector)
09:00	**Mechanistic understanding of N2 activation: a comparison of unsupported and supported Ru catalysts** Hsin-Yi Tiffany Chen *National Tsing Hua University, Chinese Taipei*
09:05	**In the search for the bottlenecks of ammonia synthesis over Ru/Vulcan under ambient conditions** Deniz Uner *Middle East Technical University, Turkey*
09:10	**Low temperature ammonia synthesis by surface protonics over metal supported catalysts** Yasushi Sekine *Waseda University, Japan*
09:15	Discussion
10:30	Refreshments
	Session 2: Enzymatic N2 activation (Session chair: Chris Pickett and Richard Catlow)
11:00	**A conformational equilibrium in the nitrogenase MoFe protein with an α-V70I amino acid substitution illuminates the mechanism of H2 formation** Lance Seefeldt *Utah State University, USA*
11:05	**Structural correlations of nitrogenase active sites using nuclear resonance vibrational spectroscopy and QM/MM calculations** Serena DeBeer* *MPI Mulheim, Germany*
11:10	**Electrochemical experiments define the potentials associated with binding of substrates and inhibitors to nitrogenase MoFe protein** Kylie Vincent *University of Oxford, UK*
11:15	Discussion
12:30	Lunch
	Session 3: Electrocatalytic and photocatalytic routes to N2 activation (Session chair: Kylie Vincent and Chris Pickett)
13:30	**Hydrogen ionic conductors and ammonia conversions** John Irvine *University of St Andrews, UK*
13:35	**Electrochemical nitrogen reduction reaction over gallium – a computational and experimental study** Vivek Sinha* *C2CAT B.V., Netherlands*
13:40	**The origin of overpotential in lithium-mediated nitrogen reduction** Olivia Westhead *Imperial College London, UK*
13:45	Discussion
15:00	Refreshments

	(Session chair: Andrew Hector and Kylie Vincent)
15:30	**Sustainable ammonia synthesis through electrochemical dinitrogen activation using Ag2VO2PO4 catalyst** Divyani Gupta *Indian Institute of Technology Ropar, India*
15:35	**Designing mixed-metal electrocatalyst systems for photoelectrochemical nitrogen activation** Katharina Brinkert *University of Warwick, UK*
15:40	**A rotating ring disc electrode study of photocatalyst for nitrogen fixation** Marta Hatzell *Georgia Institute of Technology, USA*
15:45	**N2 solar activation: ammonia as hydrogen vector for energy storage** Lorenzo Rizzato *University of Padova, Italy*
15:50	Discussion
17:30	Close of sessions
19:00	Pre-dinner drinks
19:30	Conference dinner

Wednesday 29 March 2023 (timings are BST)

	Session 4: Homogeneous N2 activation (Session chair: Chris Pickett and Justin Hargreaves)
09:00	**Catalytic reduction of dinitrogen to ammonia using porphyrin-molybdenum catalysts** Patrick Holland *Yale, USA*
09:05	**Advancing electrocatalytic nitrogen fixation: insights from molecular systems** Jonas Peters *CalTech, USA*
09:10	**Plasma-based ammonia synthesis: the knowns and unknowns** Xin Zeng* *Institute of Electrical Engineering Chinese Academy of Sciences, China*
09:15	Discussion
10:30	Refreshments
	Session 5: Alternative routes to NH3 and its application (Session chair: Justin Hargreaves and Ping Chen)
11:00	**Why copper catalyzes electrochemical reduction of nitrate to ammonia** Samira Siahrostami *University of Calgary, Canada*
11:05	**Metal-loaded zeolites in ammonia decomposition catalysis** Edman Tsang* *University of Oxford, UK*
11:10	Discussion
12:00	**Concluding remarks lecture** (Session chair: Andrew Hector and Richard Catlow) Douglas MacFarlane *Monash University, Australia*
12:45	**Acknowledgements**
13:00	Close of meeting and lunch

*presenting online

Following the close of the conference the online platform and poster platform will remain open for delegates to continue networking.