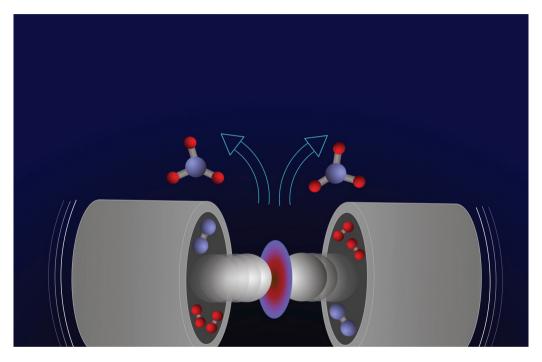
Sustainable Nitrogen Activation

Burlington House, London, UK and online 27th-29th March 2023



FARADAY DISCUSSIONS Volume 243, 2023

ROYAL SOCIETY OF CHEMISTRY The Faraday Community for Physical Chemistry of the Royal Society of Chemistry, previously the Faraday Society, was founded in 1903 to promote the study of sciences lying between chemistry, physics and biology.

Editorial Staff

Executive Editor

Michael A. Rowan

Deputy Editor Vikki Pritchard

Development Editors

Bee Hockin, Andrea Carolina Ojeda Porras

Editorial Production Manager

Gisela Scott

Senior Publishing Editor Robin Brabham

Publishing Editor

Callum woor

Editorial Assistant Daphne Houston

Publishing Assistants

Lee Colwill, Natalie Ford

Publisher

Jeanne Andres

Faraday Discussions (Print ISSN 1359-6640,

Electronic ISSN 1364-5498) is published 8 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

Volume 243 ISBN 978-1-83767-090-1

2023 annual subscription price: print+electronic £1223

US \$2154; electronic only £1165, US \$2051.

Customers in Canada will be subject to a surcharge to cover GST.

Customers in the EU subscribing to the electronic version only will be charged VAT.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail orders@rsc.org

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Printed in the UK





Faraday Discussions

Faraday Discussions are unique international discussion meetings that focus on rapidly developing areas of chemistry and its interfaces with other scientific disciplines.

Scientific Committee volume 243

Chair

Justin Hargreaves, University of Glasgow, UK

Richard Catlow, Cardiff University and University College London, UK Ping Chen, Dalian Institute of Chemical Physics, China Andrew Hector, University of Southampton, UK Christopher Pickett, University of East Anglia, UK Kylie Vincent, University of Oxford, UK

Faraday Standing Committee on Conferences

Chair

Susan Perkin, University of Oxford, UK

Secretary

Susan Weatherby, Royal Society of Chemistry, UK

George Booth, King's College London, UK Rachel Evans, University of Cambridge, UK David Fermin, University of Bristol, UK Dwayne Heard, University of Leeds, UK David Lennon, University of Glasgow,

Angelos Michaelides, University College London, UK Julia Weinstein, University of Sheffield, UK

Advisory Board

Vic Arcus, The University of Waikato, New Zealand

Timothy Easun, Cardiff University, UK Dirk Guldi, University of Erlangen-

Nuremberg, Germany Marina Kuimova, Imperial College London. UK

Luis Liz-Marzán, CIC biomaGUNE, Spain Andrew Mount, University of

Edinburgh, UK Frank Neese, Max Planck Institute for Chemical Energy Conversion, Germany Michel Orrit, Leiden University, The Netherlands

Zhong-Qun Tian, Xiamen University, China Siva Umapathy, Indian Institute of

Science, Bangalore, India Bert Weckhuysen, Utrecht University, The Netherlands

Julia Weinstein, University of Sheffield, UK

Sihai Yang, University of Manchester, UK

Information for Authors

This journal is © the Royal Society of Chemistry 2023 Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

⊕ The paper used in this publication meets the requirements of ANSI/NISO Z39.48–1992 (Permanence of Paper).

Registered charity number: 207890

Sustainable Nitrogen **Activation**

Faraday Discussions

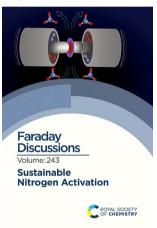
www.rsc.org/faraday d

A General Discussion on Sustainable Nitrogen Activation was held in London, UK and online on the 27th, 28th and 29th of March 2023.

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

CONTENTS

ISSN 1359-6640; ISBN 978-1-83767-090-1



Cover

See Sievers et al., Faraday Discuss., 2023, **243**, 65-76.

A titanium nitride catalyst is synthesized mechanochemically in a vibratory mill. Collisions alter material properties and produce favorable reaction conditions for ammonia synthesis.

Image reproduced with permission of Jacob A. DeWitt and Carsten Sievers from Sievers et al., Faraday Discuss., 2023. **243**. 65-76.

INTRODUCTORY LECTURE

Spiers Memorial Lecture: Catalytic activation of molecular nitrogen for green ammonia synthesis: introduction and current status Hideo Hosono

PAPERS AND DISCUSSIONS

- Barium hydride activates Ni for ammonia synthesis catalysis Wenbo Gao, Qianru Wang, Yeqin Guan, Hanxue Yan, Jianping Guo and Ping Chen
- Ionic conductivity and disorder in calcium and barium nitrogen hydrogen phases Gavin J. Irvine and John T. S. Irvine
- The formation of a lithium-iridium complex hydride toward ammonia synthesis Hanxue Yan, Wenbo Gao, Qianru Wang, Jianping Guo and Ping Chen







- Structural evolution of TiN catalysts during mechanocatalytic ammonia synthesis Jacob A. DeWitt, Erin V. Phillips, Karoline L. Hebisch, Andrew W. Tricker and Carsten Sievers
- Mechanism of ammonia synthesis on Fe₃Mo₃N Michael D. Higham, Constantinos D. Zeinalipour-Yazdi, Justin S. J. Hargreaves and C. Richard A. Catlow
- 97 Experimental and theoretical investigations on the anti-perovskite nitrides Co_zCuN. Ni₃CuN and Co₃MoN for ammonia synthesis Angela Daisley, Michael Higham, C. Richard A. Catlow and Justin S. J. Hargreaves
- 126 Switching on/off molybdenum nitride catalytic activity in ammonia synthesis through modulating metal-support interaction Amanda Sfeir, Camila A. Teles, Maya Marinova, Hérve Vezin, Jean-Philippe Dacquin, Axel Löfberg, Said Laassiri and Sébastien Rover
- 148 Mechanistic understanding of N₂ activation: a comparison of unsupported and supported Ru catalysts Yves Ira A. Reyes, Kai-Shiang Yang, Ho Viet Thang, Carmine Coluccini, Shih-Yuan Chen and Hsin-Yi Tiffany Chen
- 164 In search of the bottlenecks of ammonia synthesis over Ru/Vulcan under ambient conditions Mustafa Y. Aslan, Ersen Mete and Deniz Uner
- Low temperature ammonia synthesis by surface protonics over metal supported catalysts 179 Yasushi Sekine
- Heterogeneous catalytic and chemical looping routes to N₂ activation: general discussion
- A conformational equilibrium in the nitrogenase MoFe protein with an α -V70I amino acid substitution illuminates the mechanism of H2 formation Dmitriy A. Lukoyanov, Zhi-Yong Yang, Krista Shisler, John W. Peters, Simone Raugei, Dennis R. Dean, Lance C. Seefeldt and Brian M. Hoffman
- Structural correlations of nitrogenase active sites using nuclear resonance vibrational spectroscopy and QM/MM calculations Casey Van Stappen, Bardi Benediktsson, Atanu Rana, Aleksandr Chumakov, Yoshitaka Yoda, Dimitrios Bessas, Laure Decamps, Ragnar Bjornsson and Serena DeBeer
- Electrochemical experiments define potentials associated with binding of substrates 270 and inhibitors to nitrogenase MoFe protein Ting Chen, Philip A. Ash, Lance C. Seefeldt and Kylie A. Vincent
- Enzymatic N₂ activation: general discussion 287
- Hydrogen ionic conductors and ammonia conversions John T. S. Irvine, Stephy Wilson, Sujitra Amnuaypanich, Gavin J. Irvine, Maarten C. Verbraeken, Kamil Nowicki and George M. Carins
- Electrochemical nitrogen reduction reaction over gallium a computational and experimental study Vivek Sinha, Fateme Rezai, Nihat Ege Sahin, Jacopo Catalano, Espen Drath Bøjesen, Farnaz Sotoodeh and Emil Dražević

- The origin of overpotential in lithium-mediated nitrogen reduction O. Westhead, R. Tort, M. Spry, J. Rietbrock, R. Jervis, A. Grimaud, A. Bagger and I. E. L. Stephens
- Sustainable ammonia synthesis through electrochemical dinitrogen activation using an Aq₂VO₂PO₄ catalyst

Divyani Gupta, Alankar Kafle and Tharamani C. Nagaiah

354 Designing mixed-metal electrocatalyst systems for photoelectrochemical dinitrogen activation

Manpreet Kaur, Marc Walker, Steven Hindmarsh, Charlotte Bolt, Stephen York, Yisong Han, Martin R. Lees and Katharina Brinkert

- 378 A rotating ring disc electrode study of photo(electro)catalyst for nitrogen fixation Yu-Hsuan Liu, Po-Wei Huang and Marta C. Hatzell
- N₂ solar activation: ammonia as a hydrogen vector for energy storage Lorenzo Rizzato, Jonathan Cavazzani, Andrea Osti and Antonella Glisenti
- 402 Electrocatalytic and photocatalytic routes to N₂ activation: general discussion
- 429 Catalytic reduction of dinitrogen to ammonia using molybdenum porphyrin complexes

Alexander S. Hegg, Brandon Q. Mercado, Alexander J. M. Miller and Patrick L. Holland

- 450 Advancing electrocatalytic nitrogen fixation: insights from molecular systems Jonas C. Peters
- 473 Recent advances in plasma-enabled ammonia synthesis: state-of-the-art, challenges, and outlook Xin Zeng, Shuai Zhang, Xiucui Hu, Cheng Zhang, Kostya (Ken) Ostrikov and Tao Shao

- 492 Homogeneous N₂ activation: general discussion
- Why copper catalyzes electrochemical reduction of nitrate to ammonia Mohammadreza Karamad, Tiago J. Goncalves, Santiago Jimenez-Villegas, Ian D. Gates and Samira Siahrostami
- Metal-loaded zeolites in ammonia decomposition catalysis Kwan Chee Leung, Ephraem Tan, Guangchao Li, Bryan Kit Yue Ng, Ping-Luen Ho, Konstantin Lebedev and Shik Chi Edman Tsang
- Alternative routes to NH₃ and its application: general discussion

CONCLUDING REMARKS

Concluding remarks: Sustainable nitrogen activation - are we there yet? Douglas R. MacFarlane, Alexandr N. Simonov, Thi Mung Vu, Sam Johnston and Luis Miguel Azofra

ADDITIONAL INFORMATION

- 571 Poster titles
- List of participants