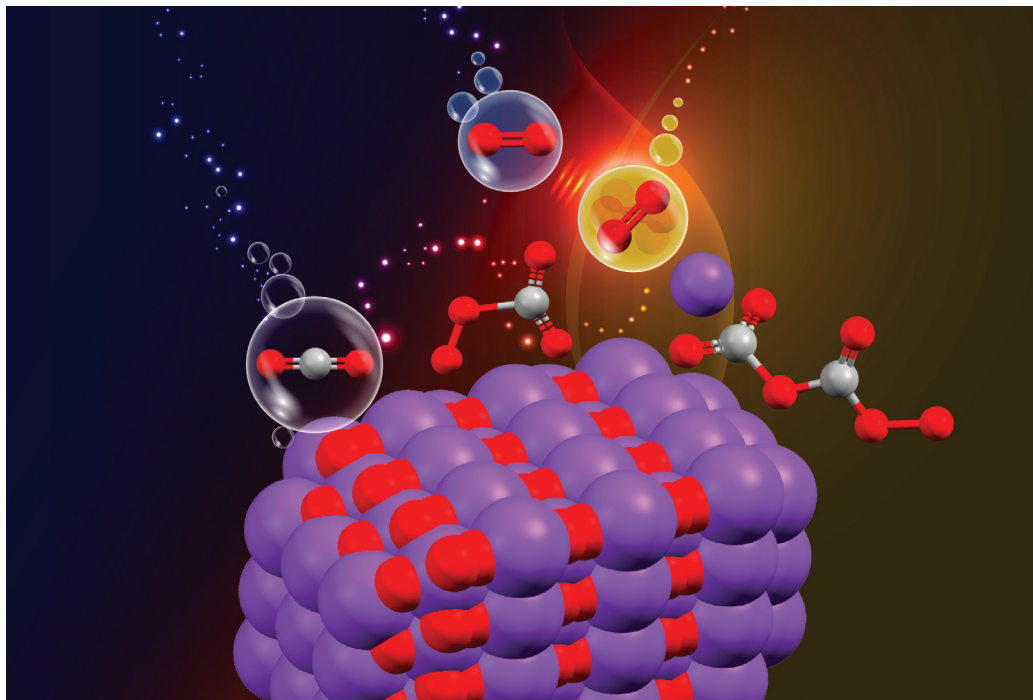


Rechargeable non-aqueous metal-oxygen batteries

York, United Kingdom

18 - 20 September 2023



FARADAY DISCUSSIONS

Volume 248, 2024



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 Editors

Michael Spenceclayh and Kate Tustain

Editorial Assistant

Daphne Houston

Publishing Assistants

Rob Griffiths and David Bishop

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 0WE.

Volume 248 ISBN 978-1-83916-427-9

2024 annual subscription price: print+electronic £1272

US \$2240; electronic only £1212, US \$2133.

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 0WE, 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 248

Chair

Laurence Hardwick, University of Liverpool, UK

Committee

Peter Bruce, University of Oxford, UK
Kristina Edstrom, Uppsala University, Sweden
Andrew Gewirth, University of Illinois at Urbana-Champaign, United States
Pooja Goddard, University of Loughborough, UK
Lee Johnson, University of Nottingham, 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, UK

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 Guld, 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 2024 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

Rechargeable non-aqueous metal-oxygen batteries

Faraday Discussions

www.rsc.org/faraday_d

A General Discussion on Rechargeable non-aqueous metal-oxygen batteries was held in York, UK and online on the 18th, 19th and 20th of September 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 978-1-83916-427-9



Cover

See Freunberger *et al.*, *Faraday Discuss.*, 2024, **248**, 175–189.

Ubiquitous superoxide in Li-air cells reacts with CO₂ to form peroxycarbonate and singlet oxygen as shown by its optical emission.

Image reproduced by permission of Stefan Freunberger from *Faraday Discuss.*, 2024, **248**, 175–189.

INTRODUCTORY LECTURE

- 9 Spiers Memorial Lecture: Lithium air batteries – tracking function and failure**
Jana B. Fritzke, James H. J. Ellison, Laurence Brazel, Gabriela Horwitz, Svetlana Menkin and Clare P. Grey

PAPERS AND DISCUSSIONS

- 29 Bio-based ether solvent and ionic liquid electrolyte for sustainable sodium–air batteries**
Pierre L. Stigliano, Nagore Ortiz-Vitoriano, Lidia Medinilla, Jason E. Bara, Juan Miguel López del Amo, Luis Lezama, Maria Forsyth, David Mecerreyes and Cristina Pozo-Gonzalo
- 48 Template assisted lithium superoxide growth for lithium–oxygen batteries**
Hsien-Hau Wang, Chengji Zhang, Jing Gao, Kah Chun Lau, Samuel T. Plunkett, Moon Park, Rachid Amine and Larry A. Curtiss



SPONSORS



POSTER SPONSOR



FARADAY COMMUNITY
FOR PHYSICAL CHEMISTRY





- 60 Feasibility of achieving two-electron K–O₂ batteries**
Lei Qin, Huiling Ao and Yiying Wu
- 75 Materials for stable metal–oxygen battery cathodes: general discussion**
- 89 K–O₂ electrochemistry at the Au/DMSO interface probed by *in situ* spectroscopy and theoretical calculations**
Jinwen Liu, Limin Guo, Ye Xu, Jun Huang and Zhangquan Peng
- 102 Effect of alkali-metal cation on oxygen adsorption at Pt single-crystal electrodes in non-aqueous electrolytes**
Julia Fernández-Vidal, Laurence J. Hardwick, Gema Cabello and Gary A. Attard
- 119 Unraveling the solvent stability on the cathode surface of Li–O₂ batteries by using *in situ* vibrational spectroscopies**
Aimin Ge, Ryuuta Nagai, Kota Nemoto, Bingbing Li, Koki Kannari, Ken-ichi Inoue and Shen Ye
- 134 A solid-state Li–air battery: computational studies of interfaces and relevance to discharge mechanism**
Nannan Shan, Anh T. Ngo, Alireza Kondari, Mohammad Asadi and Larry A. Curtiss
- 145 Solvent-dependent iodide interactions in LiO₂ electrolytes – a molecular dynamics study**
Erlendur Jónsson, Astrid H. Berge, Clare P. Grey and Israel Temprano
- 160 Dissolved LiO₂ or adsorbed LiO₂? The reactive superoxide during discharging process in lithium–oxygen batteries**
Chuan Tan, Wentao Wang, Yuping Wu and Yuhui Chen
- 175 Singlet oxygen formation in non-aqueous oxygen redox chemistry: direct spectroscopic evidence for formation pathways and reliability of chemical probes**
Soumyadip Mondal, Rajesh B. Jethwa, Bhargavi Pant, Robert Hauschild and Stefan A. Freunberger
- 190 *Operando* detection and suppression of spurious singlet oxygen in Li–O₂ batteries**
Daniel Córdoba, Leandro N. Benavides, Daniel H. Murgida, Hernan B. Rodríguez and Ernesto J. Calvo
- 210 Mechanism of ORR and OER in non-aqueous electrolytes: general discussion**
- 250 Effect of depth of discharge (DOD) on cycling *in situ* formed Li anodes**
Kiwoong Lee and Jeff Sakamoto
- 266 Toward solid-state Li_{metal}–air batteries; an SOFC perspective of solid 3D architectures, heterogeneous interfaces, and oxygen exchange kinetics**
Eric D. Wachsman, George V. Alexander, Roxanna Moores, Gibson Scisco, Christopher R. Tang and Michael Danner
- 277 Insights into soft short circuit-based degradation of lithium metal batteries**
Svetlana Menkin, Jana B. Fritzke, Rebecca Larnier, Cas de Leeuw, Yoonseong Choi, Anna B. Gunnarsdóttir and Clare P. Grey
- 298 Metal anodes and protected interfaces: general discussion**

- 305 Self-sufficient metal–air battery systems enabled by solid-ion conductive interphases**
Shuo Jin, Shifeng Hong, Xiaosi Gao, Yue Deng, Yong Lak Joo and Lynden A. Archer
- 318 The accumulation of Li_2CO_3 in a $\text{Li}-\text{O}_2$ battery with dual mediators**
Max Jenkins, Daniel Dewar, Tammy Nimmo, Chloe Chau, Xiangwen Gao and Peter G. Bruce
- 327 A facile coprecipitation approach for synthesizing $\text{LaNi}_{0.5}\text{Co}_{0.5}\text{O}_3$ as the cathode for a molten-salt lithium–oxygen battery**
Qianyuan Qiu, Jiaqi Wang, Penghui Yao and Yongdan Li
- 341 Evaluation of performance metrics for high energy density rechargeable lithium–oxygen batteries**
Shoichi Matsuda, Eiki Yasukawa, Shin Kimura, Shoji Yamaguchi and Kohei Uosaki
- 355 Engineering considerations for practical lithium–air electrolytes**
James H. J. Ellison and Clare P. Grey
- 381 A lithium–air battery and gas handling system demonstrator**
Jack W. Jordan, Ganesh Vailaya, Conrad Holc, Max Jenkins, Rory C. McNulty, Constantin Puscalau, Begum Tokay, Andrea Laybourn, Xiangwen Gao, Darren A. Walsh, Graham N. Newton, Peter G. Bruce and Lee R. Johnson
- 392 Towards practical metal–oxygen batteries: general discussion**

CONCLUDING REMARKS

- 412 Concluding remarks: a summary of the *Faraday Discussion* on rechargeable non-aqueous metal–oxygen batteries**
Laurence J. Hardwick

ADDITIONAL INFORMATION

- 423 Poster titles**
- 425 List of participants**

