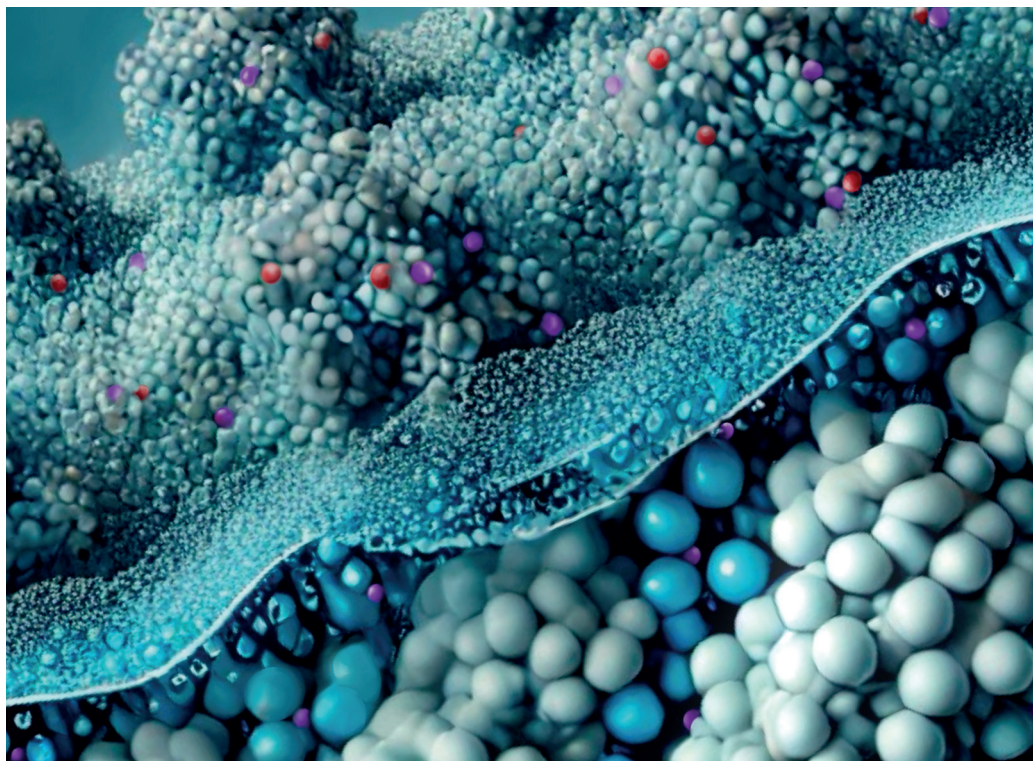


Dense Ionic Fluids

Burlington House,
London, United Kingdom
and online

8–10 July 2024



FARADAY DISCUSSIONS

Volume 253, 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

Edward Gardner

Development Editors

Bee Hockin, Andrea Carolina Ojeda-Porras

Editorial Manager

Gisela Scott

Associate Editorial Manager

Chris Goodall

Publishing Editors

Catherine Au and Harriet Brewerton

Editorial Assistant

Daphne Houston

Publishing Assistants

Huw Hedges and Julie-Ann Roszkowski

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 253 ISBN 978-1-83767-389-6

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 253

Co-Chairs

Tom Welton, Imperial College
London, UK

Susan Perkin, University of Oxford,
UK

Committee

Andrew Abbott, University of
Leicester, UK

Patricia Hunt, Victoria University of
Wellington, New Zealand
Benjamin Rotenberg, Sorbonne
Université, France

Masayoshi Watanabe, Yokohoma
National University, Japan

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

Julia Lehman, University of
Birmingham, UK

David Lennon, University of Glasgow,
UK

Andrew Mount, University of
Edinburgh, 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 Umaphathy, 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

Dense Ionic Fluids

Faraday Discussions

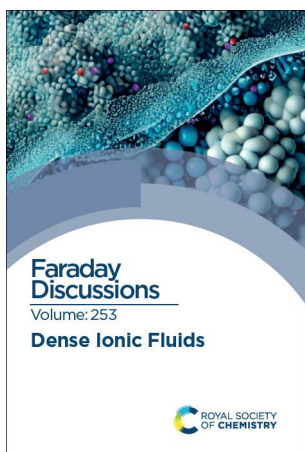
www.rsc.org/faraday_d

A General Discussion on Dense Ionic Fluids was held in London, UK and online on the 8th, 9th and 10th of July 2024.

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 978-1-83767-389-6



Cover

See Paola Carbone *et al.*, *Faraday Discuss.*, 2024, **253**, 212–232.

What drives phase separation in water-based electrolytes?

Image reproduced with permission of Hannah O. Wood from Paola Carbone *et al.*, *Faraday Discuss.*, 2024, **253**, 212–232.

PREFACE

9

Preface

Susan Perkin and Tom Welton

INTRODUCTORY LECTURE

11

Spiers Memorial Lecture: From cold to hot, the structure and structural dynamics of dense ionic fluids

Matthew S. Emerson, Raphael Ogbodo and Claudio J. Margulis

PAPERS AND DISCUSSIONS

26

Cationic micelles in deep eutectic solvents: effects of solvent composition

Iva Manasi, Stephen M. King and Karen J. Edler

42

Speciation and dipole reorientation dynamics of glass-forming liquid electrolytes: Li [N(SO₂CF₃)₂] mixtures of 1,3-propane sultone or tetrahydrothiophene-1,1-dioxide

Yasuhiro Umabayashi, Erika Otani, Hikari Watanabe and Jihae Han



POSTER SPONSOR



SPONSORS

IOP | Institute of Physics
Thin Films and Surfaces Group

EXHIBITORS





- 55 Chain-length dependent organisation in mixtures of hydrogenous and fluorous ionic liquids**
Naomi S. Elstone, Emily V. Shaw, Karina Shimizu, Joshua Lai, Bruno Demé, Paul D. Lane, Matthew L. Costen, Kenneth G. McKendrick, Sarah Youngs, Sarah E. Rogers, Jose N. Canongia Lopes, Duncan W. Bruce and John M. Slattery
- 79 Chemical models for dense solutions**
J.-F. Dufrêche, B. Siboulet and M. Duvail
- 100 Overdetermination method for accurate dynamic ion correlations in highly concentrated electrolytes**
Tabita Pothmann, Maleen Middendorf, Christian Gerken, Pinchas Nürnberg, Monika Schönhoff and Bernhard Roling
- 118 Exploring the structure of type V deep eutectic solvents by xenon NMR spectroscopy**
Matteo Boveni, Michele Mauri, Franca Castiglione and Roberto Simonutti
- 129 Machine learning-driven investigation of the structure and dynamics of the BMIM-BF₄ room temperature ionic liquid**
Fabian Zills, Moritz René Schäfer, Samuel Tovey, Johannes Kästner and Christian Holm
- 146 Structure and dynamics in dense ionic fluids: general discussion**
- 181 Revisiting the driving force inducing phase separation in PEG–phosphate aqueous biphasic systems**
Sophie Bonnassieux, Raj Pandya, Dhyllan Adan Skiba, Damien Degoulange, Dorothee Petit, Peter Seem, Russel P. Cowburn, Betar M. Gallant and Alexis Grimaud
- 193 Wave mechanics in an ionic liquid mixture**
Timothy S. Groves and Susan Perkin
- 212 Stability and structure of the aqueous LiTFSI–LiCl interface**
Hannah O. Wood, Hannah M. Burnett, Robert A. W. Dryfe and Paola Carbone
- 233 Tailored carbon dioxide capacity in carboxylate-based ionic liquids**
Nicolas Scaglione, Jocasta Avila, Agilio Padua and Margarida Costa Gomes
- 251 Unravelling the complex speciation of halozincate ionic liquids using X-ray spectroscopies and calculations**
J. M. Seymour, E. Gousseva, F. K. Towers Tompkins, L. G. Parker, N. O. Alblewi, C. J. Clarke, S. Hayama, R. G. Palgrave, R. A. Bennett, R. P. Matthews and K. R. J. Lovelock
- 273 Deep eutectic solvents on a tightrope: balancing the entropy and enthalpy of mixing**
Adriaan van den Bruinhorst, Chiara Corsini, Guillaume Depraetere, Nithavong Cam, Agilio Pádua and Margarida Costa Gomes
- 289 Ionic fluids at equilibrium: thermodynamics, nanostructure, phase behaviour, activity: general discussion**
- 314 Stabilization of lithium metal in concentrated electrolytes: effects of electrode potential and solid electrolyte interphase formation**
Anusha Pradhan, Shoma Nishimura, Yasuyuki Kondo, Tomoaki Kaneko, Yu Katayama, Keitaro Sodeyama and Yuki Yamada

- 329 Overcoming passivation through improved mass transport in dense ionic fluids**
Evangelia Daskalopoulou, Philip Hunt, Christopher E. Elgar, Minjun Yang, Andrew P. Abbott and Jennifer M. Hartley
- 343 Heterogeneous Li coordination in solvent-in-salt electrolytes enables high Li transference numbers**
Anne Hockmann, Florian Ackermann, Diddo Diddens, Isidora Cekic-Laskovic and Monika Schönhoff
- 365 Electric field induced associations in the double layer of salt-in-ionic-liquid electrolytes**
Daniel M. Markiewitz, Zachary A. H. Goodwin, Michael McEldrew, J. Pedro de Souza, Xuhui Zhang, Rosa M. Espinosa-Marzal and Martin Z. Bazant
- 385 Linear ether-based highly concentrated electrolytes for Li–sulfur batteries**
Toru Ishikawa, Shohei Haga, Keisuke Shigenobu, Taku Sudoh, Seiji Tsuzuki, Wataru Shinoda, Kaoru Dokko, Masayoshi Watanabe and Kazuhide Ueno
- 407 Ionic fluids out of equilibrium: electrodeposition, dissolution, electron transfer, driving forces: general discussion**
- 426 Ion transport in polymerized ionic liquids: a comparison of polycation and polyanion systems**
Javad Jeddi, Jukka Niskanen, Benoît H. Lessard and Joshua Sangoro
- 441 Dispersions of magnetic nanoparticles in water/ionic liquid mixtures**
T. Fiuza, M. Sarkar, J. Riedl, F. Cousin, G. Demouchy, J. Depeyrot, E. Dubois, R. Perzynski and V. Peyre
- 458 Observation of cavitation dynamics in viscous deep eutectic solvents during power ultrasound sonication**
Ben Jacobson, Shida Li, Paul Daly, Christopher E. Elgar, Andrew P. Abbott, Andrew Feeney and Paul Prentice
- 478 Speciation of the proton in water-in-salt electrolytes**
Kateryna Goloviznina, Alessandra Serva and Mathieu Salanne
- 493 New directions in experiment and theory, interfaces, and interactions: general discussion**

CONCLUDING REMARKS

- 510 Concluding remarks: Dense ionic fluids: because sometimes, more is more**
Rob Atkin

ADDITIONAL INFORMATION

- 524 Poster titles**
- 526 List of participants**

