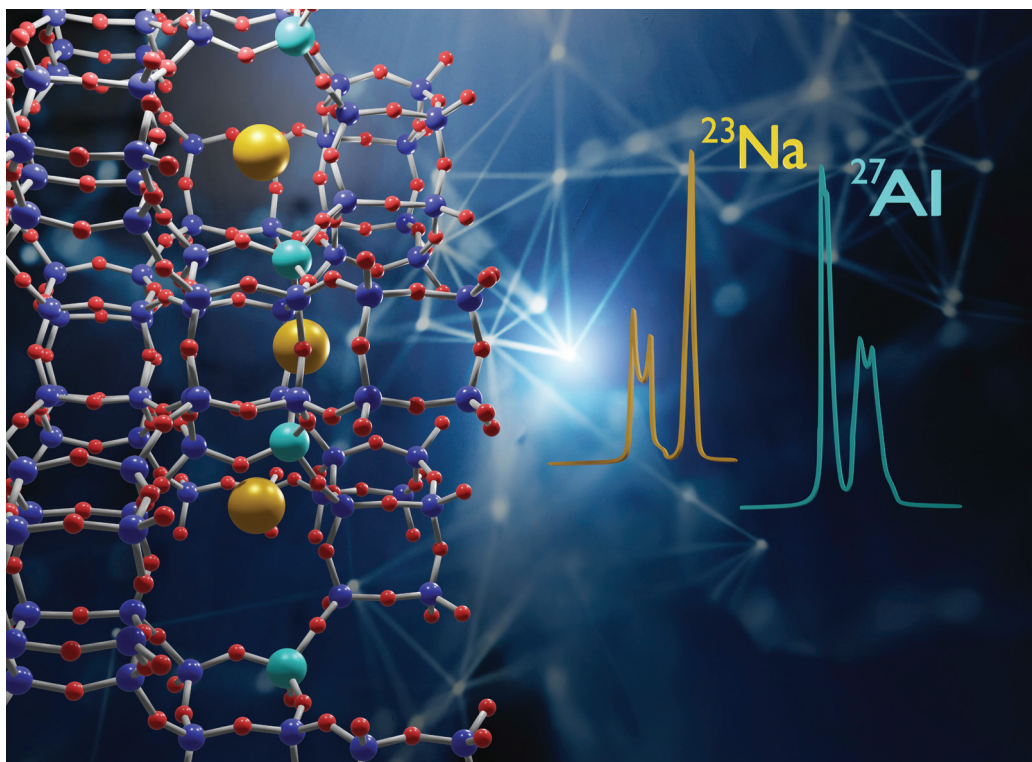


NMR Crystallography

Alan Walters Building, Birmingham,
United Kingdom and online

4-6 September 2024



FARADAY DISCUSSIONS

Volume 255, 2025

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 Coordinator

Konoya Das

Publishing Editors

Sam Mansell and Kate Tustain

Editorial Assistant

Daphne Houston

Publishing Assistants

Natalie Ford and Julie-Ann Roszkowski

Publisher

Sam Keltie

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 255 ISBN 978-1-83767-441-1

2025 annual subscription price: print+electronic £1342
US \$2363; electronic only £1279, US \$2250.
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 255

Co-Chairs

John Griffin, Lancaster University, UK
Andrew Morris, University of Birmingham, UK

Committee

David Bryce, University of Ottawa, Canada
Martin Dracinsky, Czech Academy of Sciences, Czech Republic
Danielle Laurencin, Institut Charles Gerhardt Montpellier, France
Sally Price, University College London, 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

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 Eastun, 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 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 2025. 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



NMR Crystallography

Faraday Discussions

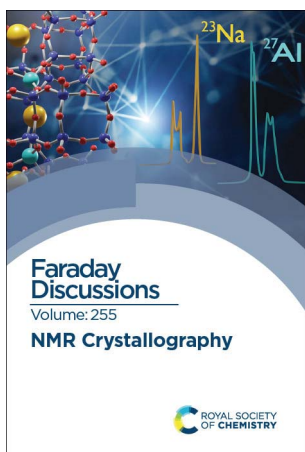
www.rsc.org/faraday_d

A General Discussion on NMR Crystallography was held in Birmingham, UK and online on 4th, 5th and 6th of September 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 978-1-83767-441-1



Cover

See Christopher J. Heard *et al.*, *Faraday Discuss.*, 2025, **255**, 46–71.

Zeolite structure alongside calculated NMR spectra.

Image reproduced with permission of Christopher J. Heard from Christopher J. Heard *et al.*, *Faraday Discuss.*, 2025, **255**, 46–71.

INTRODUCTORY LECTURE

- 9 Spiers Memorial Lecture: NMR crystallography**
Lyndon Emsley

PAPERS AND DISCUSSIONS

- 46 A machine learning approach for dynamical modelling of Al distributions in zeolites via $^{23}\text{Na}/^{27}\text{Al}$ solid-state NMR**
Chen Lei, Carlos Bornes, Oscar Bengtsson, Andreas Erlebach, Ben Slater, Lukas Grajciar and Christopher J. Heard
- 72 High-throughput calculations and machine learning modeling of ^{17}O NMR in non-magnetic oxides**
Zhiyuan Li, Bo Zhao, Hongbin Zhang and Yixuan Zhang



SPONSORS

Open Access Article, Published on 10 January 2025, Downloaded on 2/18/2025 11:23:52 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.



JEOL 

NMR 
SERVICE

ePROBE

BATTERY ANALYSIS TECHNOLOGY SOLUTIONS

POSTER SPONSOR



ROYAL SOCIETY
OF **CHEMISTRY**

FARADAY COMMUNITY
FOR PHYSICAL CHEMISTRY



- 88 Characterization of ephedrine HCl and pseudoephedrine HCl using quadrupolar NMR crystallography guided crystal structure prediction**
Carl H. Fleischer, III, Sean T. Holmes, Kirill Levin, Stanislav L. Veinberg and Robert W. Schurko
- 119 The interplay of density functional selection and crystal structure for accurate NMR chemical shift predictions**
Sebastian A. Ramos, Leonard J. Mueller and Gregory J. O. Beran
- 143 Crystal structure validation of verinurad via proton-detected ultra-fast MAS NMR and machine learning**
Daria Torodii, Jacob B. Holmes, Pinelopi Moutzouri, Sten O. Nilsson Lill, Manuel Cordova, Arthur C. Pinon, Kristof Grohe, Sebastian Wegner, Okky Dwichandra Putra, Stefan Norberg, Anette Welinder, Staffan Schantz and Lyndon Emsley
- 159 Big data and simulations in NMR crystallography: general discussion**
- 192 Accurate predictions of chemical shifts with the rSCAN and r²SCAN mGGA exchange–correlation functionals**
Jonathan R. Yates and Albert P. Bartók
- 203 Uniform chi-squared model probabilities in NMR crystallography**
Leonard J. Mueller
- 222 Organic NMR crystallography: enabling progress for applications to pharmaceuticals and plant cell walls**
Zainab Rehman, Jairah Lubay, W. Trent Franks, Albert P. Bartók, Emily K. Corlett, Bao Nguyen, Garry Scrivens, Brian M. Samas, Heather Frericks-Schmidt and Steven P. Brown
- 244 Combined ⁷Li NMR, density functional theory and *operando* synchrotron X-ray powder diffraction to investigate a structural evolution of cathode material LiFeV₂O₇**
Taiana L. E. Pereira, Jon Serrano Sevillano, Beatriz D. Moreno, Joel W. Reid, Dany Carlier and Gillian R. Goward
- 266 The EFG Rosetta Stone: translating between DFT calculations and solid state NMR experiments**
Javier Valenzuela Reina, Federico Civaia, Angela F. Harper, Christoph Scheurer and Simone S. Köcher
- 288 Challenges and opportunities for NMR calculations: general discussion**
- 311 When can we trust structural models derived from pair distribution function measurements?**
Phillip M. Maffettone, William J. K. Fletcher, Thomas C. Nicholas, Volker L. Deringer, Jane R. Allison, Lorna J. Smith and Andrew L. Goodwin
- 325 The essential synergy of MD simulation and NMR in understanding amorphous drug forms**
Jamie L. Guest, Esther A. E. Bourne, Martin A. Screen, Mark R. Wilson, Tran N. Pham and Paul Hodgkinson

- 342 **Atomic-level structure of the amorphous drug atuliflapon via NMR crystallography**
Jacob B. Holmes, Daria Torodii, Martins Balodis, Manuel Cordova, Albert Hofstetter, Federico Paruzzo, Sten O. Nilsson Lill, Emma Eriksson, Pierrick Berruyer, Bruno Simões de Almeida, Mike Quayle, Stefan Norberg, Anna Svensk Ankarberg, Staffan Schantz and Lyndon Emsley
- 355 **Investigating the effect of particle size distribution and complex exchange dynamics on NMR spectra of ions diffusing in disordered porous carbons through a mesoscopic model**
El Hassane Lahrar and Céline Merlet
- 370 **First-principles NMR of oxide glasses boosted by machine learning**
Thibault Charpentier
- 391 **Generating models that describe complex disorder: general discussion**
- 411 **Tracking Li atoms in real-time with ultra-fast NMR simulations**
Angela F. Harper, Tabea Huss, Simone S. Köcher and Christoph Scheurer
- 429 **Metastable layered lithium-rich niobium and tantalum oxides via nearly instantaneous cation exchange**
Sarah L. Ko, Jordan A. Dorrell, Andrew J. Morris and Kent J. Griffith
- 451 **Temperature-induced mobility in octacalcium phosphate impacts crystal symmetry: water dynamics studied by NMR crystallography**
Adam Nelson, Wassilios Papawassiliou, Subhradip Paul, Sabine Hediger, Ivan Hung, Zhehong Gan, Amrit Venkatesh, W. Trent Trent Franks, Mark E. Smith, David Gajan, Gaël De Paëpe, Christian Bonhomme, Danielle Laurencin and Christel Gervais
- 483 **Exploring the crystallisation of aspirin in a confined porous material using solid-state nuclear magnetic resonance**
Marie Juramy, Eric Besson, Stéphane Gastaldi, Fabio Ziarelli, Stéphane Viel, Giulia Mollica and Pierre Thureau
- 495 **Probing assembly/disassembly of ordered molecular hydrogels**
Susana M. Ramalheite, Karol P. Nartowski, Hayley Green, Jesús Angulo, Dinu Iuga, László Fábrián, Gareth O. Lloyd and Yaroslav Z. Khimyak
- 520 **NMR crystallization: *in situ* NMR strategies for monitoring the evolution of crystallization processes**
Colan E. Hughes, Naomi V. Ratnasingam, P. Andrew Williams, Erwan Benhenou, Rhian Patterson and Kenneth D. M. Harris
- 553 **Understanding dynamics and mechanisms: general discussion**

CONCLUDING REMARKS

- 583 **Concluding remarks: *Faraday Discussion* on NMR crystallography**
Sharon E. Ashbrook

ADDITIONAL INFORMATION

- 602 **Poster titles**
- 604 **List of participants**

