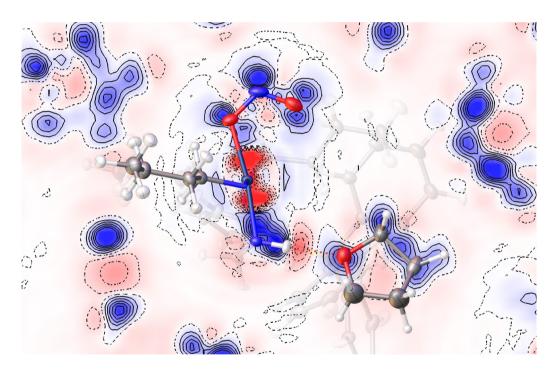
# Harnessing non-covalent interactions for synthesis and catalysis

National Stem Learning Centre, York, UK and online 12th-14th April 2023



# **FARADAY DISCUSSIONS**

Volume 244, 2023



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** 

Emily Cuffin-Munday, Claire Mitchell, Michael Whitelaw

**Editorial Assistant** 

Daphne Houston

**Publishing Assistants** 

Lee Colwill, Rob Griffiths

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 244 ISBN 978-1-83767-091-8

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 244

Andrew Weller, University of York, UK Paul Raithby, University of Bath, UK Neil Champness, University of Birmingham, UK Anne Duhme-Klair, University of York, UK Joost Reek, University of Amsterdam, Netherlands

#### Faraday Standing Committee on Conferences

Susan Perkin, University of Oxford,

#### 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,

Dwayne Heard, University of Leeds,

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

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,

Michel Orrit, Leiden University, The Netherlands

Timothy Easun, Cardiff University, UK Zhong-Qun Tian, Xiamen University, China

> Siva Umapathy, Indian Institute of Science, Bangalore, India Bert Weckhuysen, Utrecht University, The Netherlands

Iulia Weinstein, University of Sheffield, UK

Sihai Yang, University of Manchester,

### 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

# Harnessing Non-Covalent Interactions for Synthesis and Catalysis

Faraday Discussions

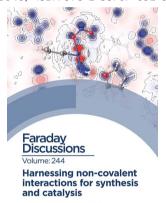
## www.rsc.org/faraday d

A General Discussion on Harnessing Non-Covalent Interactions for Synthesis and Catalysis was held in York, UK and online on the 12<sup>th</sup>, 13<sup>th</sup> and 14<sup>th</sup> of April 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 978-1-83767-091-8



ROYAL SOCIETY OF CHEMISTRY

#### Cover

See Hatcher et al., Faraday Discuss., 2023, 244, 370-390.

Uncovering the hidden noncovalent interactions that affect small molecule photoswitching using non-spherical atom refinements in NoSpherA2.

Image reproduced by permission of Lauren Hatcher from Faraday Discuss., 2023, 244, 370-390.

## INTRODUCTORY LECTURE

Spiers Memorial Lecture: Shielding the active site: a streptavidin superoxidedismutase chimera as a host protein for asymmetric transfer hydrogenation Nico V. Igareta, Ryo Tachibana, Daniel C. Spiess, Ryan L. Peterson and Thomas R. Ward

#### PAPERS AND DISCUSSIONS

Fine-tuning non-covalent interactions between hybrid metal-oxo clusters and

Sarah Lentink, David E. Salazar Marcano, Mhamad Aly Moussawi, Laurens Vandebroek, Luc Van Meervelt and Tatjana N. Parac-Vogt

(cc) BY





- 39 Effect of liquid confinement on regioselectivity in the hydrosilylation of alkynes with cationic Rh(ı) N-heterocyclic carbene catalysts
  Pradeep K. R. Panyam and Michael R. Buchmeiser
- 51 Site-selective methylene C–H oxidation of an alkyl diamine enabled by supramolecular recognition using a bioinspired manganese catalyst Arnau Vicens, Laia Vicens, Giorgio Olivo, Osvaldo Lanzalunga, Stefano Di Stefano and Miquel Costas
- 62 Solution and solid-state studies of hydrogen and halogen bonding with Nheterocyclic carbene supported nickel(II) fluoride complexes Vargini G. Thangavadivale, Lukas Tendera, Rüdiger Bertermann, Udo Radius, Torsten Beweries and Robin N. Perutz
- 77 Chalcogen bonding in copper(II)-mediated synthesis
  Vusala A. Aliyeva, Atash V. Gurbanov, Abdallah G. Mahmoud, Rosa M. Gomila,
  Antonio Frontera, Kamran T. Mahmudov and Armando J. L. Pombeiro
- 96 Manipulate techniques to manipulate the surroundings of a synthetic catalyst to control activity and selectivity: general discussion
- Catalytic templated length-controlled oligomerization
  Bartosz Lewandowski, Rebecca J. B. Schäfer, Etienne Cotter, Dora Harangozo
  and Helma Wennemers
- The bridge towards a more stable and active side-on-peroxido ( $Cu_2^{II}(\mu-\eta^2:\eta^2-O_2)$ ) complex as a tyrosinase model system
  Rosalie Dalhoff, Regina Schmidt, Lena Steeb, Kristina Rabatinova, Matthias Witte, Simon Teeuwen, Salim Benjamaâ, Henrika Hüppe, Alexander Hoffmann and Sonja Herres-Pawlis
- On the mechanism of intermolecular nitrogen-atom transfer from a lattice-isolated diruthenium nitride intermediate

Mario N. Cosio, Waad S. Alharbi, Aishanee Sur, Chen-Hao Wang, Ahmad Najafian, Thomas R. Cundari and David C. Powers

- A substrate descriptor based approach for the prediction and understanding of the regioselectivity in caged catalyzed hydroformylation

  Pim R. Linnebank, David A. Poole, Alexander M. Kluwer and Joost N. H. Reek
- Boosting the activity of Mizoroki–Heck cross-coupling reactions with a supramolecular palladium catalyst favouring remote Zn…pyridine interactions Naba Abuhafez and Rafael Gramage-Doria
- Probing the influence of substrate binding on photocatalytic dehalogenation with a heteroleptic supramolecular [M<sub>4</sub>L<sup>a</sup><sub>2</sub>L<sup>b</sup><sub>2</sub>] square containing PDI photosensitizers as ligands
  - C. Jasslie Nielsen, Petrus C. M. Laan, Raoul Plessius, Joost N. H. Reek, Jarl Ivar van der Vlugt and Sonja Pullen
- 210 Measure understanding of structural and electronic changes occurring within the relevant timescale of catalytic systems: general discussion
- A comparison of non-covalent interactions in the crystal structures of two  $\sigma$ -alkane complexes of Rh exhibiting contrasting stabilities in the solid state

  M. Arif Sajjad, Stuart A. Macgregor and Andrew S. Weller

241	Catalytic activation via $\pi$ -backbonding in halogen bonds
	Andrew Wang and Pierre Kennepohl

- H-Bonding leading to latent initiators for olefin metathesis polymerization Artur Brotons-Rufes, Naeimeh Bahri-Laleh and Albert Poater
- 269 Mapping the photochemistry of cyclopentadiene: from theory to ultrafast X-ray scattering

  Lauren Bertram, Peter M. Weber and Adam Kirrander
- 204 Alle Provided and advantage to the characteristic and a second and
- Alkali metal···methyl short contacts in aluminates: more than agostic interactions Jesús Damián, Christian Rentero, Jorge Echeverría and Marta E. G. Mosquera
- Machine-learning based prediction of small molecule—surface interaction potentials lan Rouse and Vladimir Lobaskin
- Model state-of-the-art modelling and computational analysis of reactive sites: general discussion
- 356 Noncovalent bonding assessment by pair distribution function Lucy K. Saunders, Daniel Irving, Philip A. Chater and Maria Diaz-Lopez
- Uncovering the role of non-covalent interactions in solid-state photoswitches by non-spherical structure refinements with NoSpherA2 Lauren E. Hatcher, Lucy K. Saunders and Ben A. Coulson
- Ultrafast electronic, infrared, and X-ray absorption spectroscopy study of Cu(i) phosphine diimine complexes

  Martin V. Appleby, Rory A. Cowin, Iona I. Ivalo, Samantha L. Peralta-Arriaga, Craig C. Robertson, Stuart Bartlett, Ann Fitzpatrick, Andrew Dent, Gabriel Karras, Sofia Diaz-Moreno, Dimitri Chekulaev and Julia. A. Weinstein
- 411 Structural modifications to platinum(II) pincer complexes resulting in changes in their vapochromic and solvatochromic properties

  Mathew J. Bryant, Sara Fuertes, Lauren E. Hatcher, Lynne H. Thomas and Paul R. Raithby
- 434 Make underpinning concepts of the synthesis of systems where non-covalent interactions are important: general discussion

#### **CONCLUDING REMARKS**

455 Concluding remarks: Harnessing non-covalent interactions for synthesis and catalysis

Andrew Weller

#### ADDITIONAL INFORMATION

- 459 Poster titles
- 461 List of participants