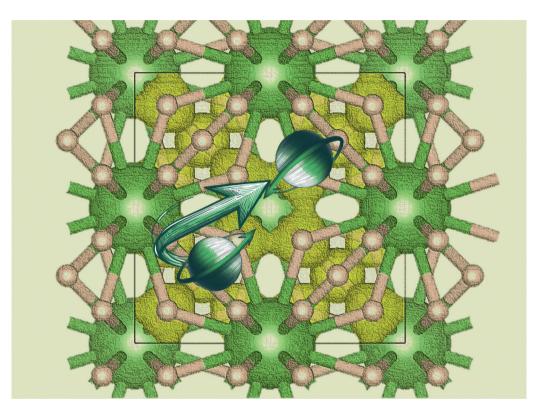
# **Correlated electronic structure** London, United Kingdom 17–19 July 2024



# **FARADAY DISCUSSIONS** Volume 254, 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** Irene Sanchez Molina, Rini Prakash and Charlotte Pugsley

Editorial Assistant Daphne Houston

**Publishing Assistants** 

Robert 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 0WF.

Volume 254 ISBN 978-1-83767-439-8

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 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

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

#### Scientific Committee volume 254

Co-Chairs George Booth, King's College London, UK Ali Alavi, Max Plank Institute Stuttgart, Germany

Committee

Peter J. Knowles, Cardiff University, UK Katarzyna Pernal, Lodz University of Technology, Poland Gustavo Scuseria, Rice University, USA Dominika Zgid, Michigan University, USA

David Fermin, University of Bristol,

David Lennon, University of Glasgow,

Julia Lehman, University of

Andrew Mount, University of

Julia Weinstein, University of

Birmingham, UK

Edinburgh, UK

Sheffield, UK

#### Faraday Standing Committee on Conferences

UK

UK

#### 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

#### Advisory Board

Vic Arcus, The University of Waikato, New Zealand Timothy Easun, Cardiff University, UK Zhong-Qun Tian, Xiamen University, 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 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, 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





# **Correlated electronic structure**

Faraday Discussions

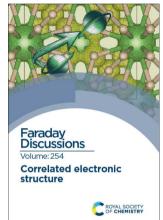
## www.rsc.org/faraday\_d

A General Discussion on Correlated electronic structure was held in London, UK and online on the  $17^{th}$ ,  $18^{th}$  and  $19^{th}$  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 978-1-83767-439-8



#### **Cover** See Julia Contreras-García *et al.,* Faraday Discuss., 2024, **254**, 598–611.

BCS correlation in real space

Image reproduced with permission of Julia Contreras-García from Julia Contreras-García *et al., Faraday Discuss.,* 2024, **254**, 598–611.

## PREFACE

**Preface** George H. Booth and Ali Alavi

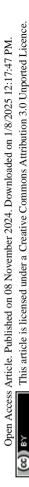
## INTRODUCTORY LECTURE

11 Spiers Memorial Lecture: Quantum chemistry, classical heuristics, and quantum advantage

Garnet Kin-Lic Chan

## PAPERS AND DISCUSSIONS

- 53 On the notion of strong correlation in electronic structure theory Brad Ganoe and James Shee
- 76 What can quantum information theory offer to quantum chemistry? Damiano Aliverti-Piuri, Kaustav Chatterjee, Lexin Ding, Ke Liao, Julia Liebert and Christian Schilling





conjugated diradicals Lujo Matasović, Hugo Bronstein, Richard H. Friend and Felix Plasser Accurate and interpretable representation of correlated electronic structure via Tensor Product Selected CI Nicole M. Braunscheidel, Arnab Bachhar and Nicholas J. Mayhall 157 Tiled unitary product states for strongly correlated Hamiltonians Huah G. A. Burton Multi-reference coupled cluster theory using the normal ordered exponential ansatz Alexander D. Gunasekera, Nicholas Lee and David P. Tew 191 Novel perturbative and variational methods for stronger correlations: general discussion 216 Challenges with relativistic GW calculations in solids and molecules Gaurav Harsha, Vibin Abraham and Dominika Zgid 239 Additions and corrections Cumulant Green's function methods for molecules Pierre-François Loos, Antoine Marie and Abdallah Ammar Permutation symmetry in spin-adapted many-body wave functions Maru Song, Ali Alavi and Giovanni Li Manni A perspective on the future of quantum chemical software: the example of the ORCA program package Frank Neese Accelerated basis-set convergence of coupled-cluster excitation energies using the density-based basis-set correction method Diata Traore, Julien Toulouse and Emmanuel Giner Spinless formulation of linearized adiabatic connection approximation and its comparison with the second order N-electron valence state perturbation theory Yang Guo and Katarzyna Pernal Striking the right balance of encoding electron correlation in the Hamiltonian and the wavefunction ansatz Kalman Szenes, Maximilian Mörchen, Paul Fischill and Markus Reiher Orbital optimisation in xTC transcorrelated methods Daniel Kats, Evelin M. C. Christlmaier, Thomas Schraivogel and Ali Alavi Towards efficient quantum computing for quantum chemistry: reducing circuit complexity with transcorrelated and adaptive ansatz techniques Erika Magnusson, Aaron Fitzpatrick, Stefan Knecht, Martin Rahm and Werner Dobrautz 429 Rapidly convergent quantum Monte Carlo using a Chebyshev projector Zijun Zhao, Maria-Andreea Filip and Alex J. W. Thom 451 Stochastic and low-scaling techniques: general discussion

Classification and quantitative characterisation of the excited states of  $\pi$ -

Edgar Josué Landinez Borda, Kenneth O. Berard, Annette Lopez and Brenda Rubenstein Force and stress calculations with a neural-network wave function for solids Yubing Qian, Xiang Li and Ji Chen Fast and accurate nonadiabatic molecular dynamics enabled through variational interpolation of correlated electron wavefunctions Kemal Atalar, Yannic Rath, Rachel Crespo-Otero and George H. Booth Stochastic and low-scaling techniques/extended systems: general discussion CO adsorption on Pt(111) studied by periodic coupled cluster theory Johanna P. Carbone, Andreas Irmler, Alejandro Gallo, Tobias Schäfer, William Z. Van Benschoten, James J. Shepherd and Andreas Grüneis Introducing electron correlation in solid-state calculations for superconducting states Wilver A. Muriel, Trinidad Novoa, Carlos Cárdenas and Julia Contreras-García Magnetic structure of a multiferroic compound: Cu<sub>2</sub>OCl<sub>2</sub> Julien Lévêgue, Elisa Rebolini, Andrés Saúl and Marie-Bernadette Lepetit Adsorption and vibrational spectroscopy of CO on the surface of MgO from periodic local coupled-cluster theory Hong-Zhou Ye and Timothy C. Berkelbach 641 Restoring translational symmetry in periodic all-orbital dynamical mean-field theory simulations Jiachen Li and Tianvu Zhu Quantum embedding for molecules using auxiliary particles – the ghost Gutzwiller Ansatz Carlos Mejuto-Zaera Correlation in extended systems: general discussion

Gaussian processes for finite size extrapolation of many-body simulations

## CONCLUDING REMARKS

708 Concluding remarks Francesco A. Evangelista

## ADDITIONAL INFORMATION

- 718 Poster titles
- 721 List of participants