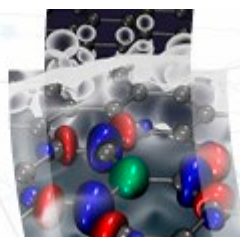


Correlated electronic structure

17–19 July 2024 | London, UK



Faraday Discussions

Wednesday 17 July 2024

11:30	Registration with lunch served from 11:45
12:45	Welcome and introductions <i>Chair of Scientific Committee</i>
12:55	Outline of Discussion format <i>Royal Society of Chemistry Publishing Editors</i>
13:00	Introductory Lecture – Spiers Memorial Lecture (Session chair: TBC) Garnet Chan <i>CalTech, USA</i>
14:00	Comfort break (no refreshments)
	Session 1: Novel perturbative and variational methods for stronger correlations (Session chair: TBC)
14:15	On the notion of strong correlation in electronic structure theory James Shee and Brad Ganoe <i>Rice University, USA</i>
14:20	What can quantum information theory offer to quantum chemistry? Christian Schilling, Damiano Aliverti-Piuri, Kaustav Chatterjee, Lexin Ding, Ke Liao, Julia Liebertab <i>LMU Munich, Germany</i>
14:25	Classification and quantitative characterisation of the excited states of π-conjugated diradicals Felix Plasser, Lujo Matasović, Hugo Bronstein, Richard H. Friend <i>Loughborough University, UK</i>
14:30	Discussion
15:45	Refreshments
	Session 1 continued: Novel perturbative and variational methods for stronger correlations (Session chair: TBC)
16:15	Accurate and interpretable representation of correlated electronic structure via tensor product selected CI Nicholas J. Mayhall, Nicole M. Braunscheidel, Arnab Bachhar <i>Virginia Tech, USA</i>
16:20	Tiled unitary product states for strongly correlated Hamiltonians Hugh G. A. Burton <i>University of Cambridge, UK</i>
16:25	Multi-reference coupled cluster theory using the normal ordered exponential ansatz Alexander Gunasekera, Nicholas Lee, David Tew <i>University of Oxford, UK</i>
16:30	Discussion
17:45	Lightning presentations – (by invitation of the Scientific Committee)
18:00	Poster session
19:30	Close

Thursday 18 July

	Session 2: Stochastic and low-scaling techniques (Session chair: TBC)
09:00	Challenges with relativistic GW calculations in solids and molecules <u>Gaurav Harsha</u> , Vibin Abraham and Dominika Zgid <i>University of Michigan Ann Arbor, USA</i>
09:05	Cumulant Green's function methods for molecules <u>Pierre-François Loos</u> , Antoine Marie and Abdallah Ammar <i>Université de Toulouse, France</i>
09:10	Permutation symmetry in spin adapted many-body wave functions <u>Giovanni Li Manni</u> , Maru Song, Ali Alavia <i>Max Planck Institute for Solid State Research, Germany</i>
09:15	Discussion
10:30	Refreshments
	Session 2 continued: Stochastic and low-scaling techniques (Session chair: TBC)
11:00	A perspective on the future of quantum chemical software: The example of the ORCA program package <u>Frank Neese</u> <i>Max-Planck-Institut für Kohlenforschung, Germany</i>
11:05	Accelerated basis-set convergence of coupled-cluster excitation energies using the density-based basis-set correction method <u>Emmanuel Giner</u> , Diata Traore, Julien Toulouse <i>CNRS, France</i>
11:10	Spinless formulation of linearized adiabatic connection approximation and its comparison with second order N-electron valence state perturbation theory <u>Yang Guo</u> and Katarzyna Pernal <i>Shandong University, China</i>
11:15	Discussion
12:30	Lunch
	Session 2 continued: Stochastic and low-scaling techniques (Session chair: TBC)
14:00	Striking the right balance of encoding electron correlation in the Hamiltonian and wavefunction ansatz <u>Markus Reiher</u> , Kalman Szenes, Maximilian Mörchen, Paul Fischill <i>ETH Zurich, Switzerland</i>
14:05	Orbital optimisation in xTC transcorrelated methods <u>Daniel Kats</u> , Evelin M. C. Christlmaier, Thomas Schraivogel, Ali Alavi <i>Max Planck Institute for Solid State Research, Germany</i>
14:10	Towards efficient quantum computing for quantum chemistry: Reducing circuit complexity with transcorrelated and adaptive ansatz techniques <u>Werner Dobrautz</u> , Erika Magnusson, Aaron Fitzpatrick, Stefan Knecht, Martin Rahm <i>Chalmers University of Technology, Sweden</i>
14:15	Rapidly convergent quantum Monte Carlo using a Chebyshev projector <u>Zijun Zhao</u> , Maria-Andreea Filip and Alex J. W. Thom <i>University of Cambridge, UK</i>
14:20	Discussion
16:00	Refreshments
	Session 3: Stochastic and low-scaling techniques / Extended systems (Session chair: TBC)
16:30	Gaussian processes for finite size extrapolation of many-body simulations <u>Brenda Rubenstein</u> , Edgar Josué Landinez Borda, Kenneth O. Berard, Annette Lopez <i>Brown University, USA</i>
16:35	Force and stress calculation with neural network wavefunction for solids <u>Ji Chen</u> , Yubing Qian, Xiang Li <i>Peking University, China</i>

16:40	Fast and accurate nonadiabatic molecular dynamics enabled through variational interpolation of correlated electron wavefunctions <u>Kemal Atalar</u> , Yannic Rath, Rachel Crespo-Otero, George H. Booth <i>King's College London, UK</i>
16:45	Discussion
18:00	Close
18:30	Pre-dinner drinks – Council Room, Burlington House
19:00	Conference dinner – Library, Burlington House

Friday 19 July

	Session 4: Correlation in extended systems (Session chair: TBC)
09:00	CO adsorption on Pt(111) studied by periodic coupled cluster theory <u>Andreas Grüneis</u> , Johanna P. Carbone, Andreas Irmmler, Alejandro Gallo, Tobias Schäfer, William Z. Van Benschoten, James J. Shepherd <i>TU Wien, Austria</i>
09:05	Introducing electron correlation in solid state calculations for superconducting states <u>Julia Contreras-García</u> , Wilver A. Muriel, <u>Trinidad Novoa</u> , Carlos Cárdenasa <i>Sorbonne University, France</i>
09:10	Magnetic structure of a multiferroic compound: Cu_2OCl_2 <u>Marie-Bernadette Lepetit</u> , Julien Lévêque, Elisa Rebolini, Andrés Saúl <i>Institut Néel, France</i>
09:15	Discussion
10:30	Refreshments
	Session 4 continued: Correlation in extended systems (Session chair: TBC)
11:00	Adsorption and vibrational spectroscopy of CO on the surface of MgO from periodic local coupled-cluster theory <u>Timothy C. Berkelbach</u> and Hong-Zhou Ye <i>Columbia University, USA</i>
11:05	Restoring translational symmetry in periodic all-orbital dynamical mean-field theory simulations <u>Tianyu Zhu</u> and Jiachen Li <i>Yale University, USA</i>
11:10	Quantum embedding for molecules with auxiliary particles - the ghost gutzwiller ansatz <u>Carlos Mejuto-Zaera</u> <i>SISSA, Italy</i>
11:15	Discussion
12:30	Concluding remarks lecture (Session chair: TBC) <u>Francesco Evangelista</u> <i>Emory University, USA</i>
13:00	Acknowledgements and presentation of poster prizes
13:15	Close of meeting and lunch

All timings are in BST

Please note that this is a draft programme and timings may change.