New horizons in density functional theory

Faraday Discussion

2–4 September 2020

All times are BST

Wednesday 2 September

13:00	**Welcome and Introductions** Andrew Teale, *Chair of Scientific Committee*
13:10	**Outline of Discussion Format** *Alexander Whiteside and Alice Coles-Aldridge* *Royal Society of Chemistry Publishing Editors*
13:15	**Introductory Lecture** (Session Chair: Andrew Teale & Emmanuel Fromager) Weitao Yang *Duke University, USA*
14:15	**Break**
	Session 1: New density-functional approximations and beyond (Session Chair: Trygve Helgaker & Paola Gori-Giorgi)
14:45	**Strategies to build functionals of the density, or functionals of Green's functions: what can we learn?** Lucia Reining, Ayoub Aouina and Matteo Gatti *École Polytechnique, France*
14:50	**Spin-state dependence of exchange-correlation holes** Christoph R Jacob and Julia Brüggemann *TU Braunschweig, Germany*
14:55	**Assessment of methods developed for the Kohn-Sham correlation energy within the framework of the adiabatic-connection-fluctuation-dissipation theorem** Jannis Erhard, Steffen Fauser, Evgeny Moerman, Simon Kalaß, Evgeny Moerman, Egor Trushin and Andreas Görling *Friedrich Alexander Universität Erlangen/Nürnberg, Germany*
15:00	Discussion
16:00	Break
	Session Chair: David Tozer & Chris Kriton-Skylaris
16:30	**Deriving approximate density functionals with asymptotics** Kieron Burke *University of California, Irvine, USA*
16:35	**Improving the exchange and correlation potential in density functional approximations through constraints** Nikitas Gidopoulos, Timothy J. Callow, Benjamin J. Pearce, Tom Pitts, Nektarios N. Lathiotakis and Matthew J. P. Hodgson *Durham University, UK*
16:40	**London dispersion forces without density distortion: a path to first principles inclusion in density functional theory** Derk Kooi and Paola Gori-Giorgi Vrije Universiteit Amsterdam, The Netherlands
16:45	Discussion
17:45	End of day

Thursday 3 September

	Session 2: Challenges for large scale simulation (Session Chair: Chris Kriton-Skylaris & Trygve Helgaker)
13:00	**Subsystem density-functional theory for interacting open-shell systems: Spin densities and magnetic exchange couplings** Johannes Neugebauer and Anja Massolle *University of Münster, Germany*
13:05	**A *posteriori error* estimation for the non-self-consistent Kohn-Sham equations** Michael Friedrich Herbst, Antoine Levitt and Eric Cancès *CERMICS, Inria Paris and Ecole des Ponts Paris Tex, France*
13:10	Discussion
13:50	Break
	Session Chair: Andrew Teale & Chris Kriton-Skylaris
14:20	**A machine learning based intramolecular potential for a flexible organic molecule** Gábor Csányi, Daniel J Cole and Letif Mones *University of Cambridge, UK*
14:25	**Insights into one-body density matrices using deep learning** Jack Wetherell, Andrea Costamagna, Matteo Gatti and Lucia Reining *École Polytechnique, France*
14:30	**Cost-effective composite methods for large scale solid-state calculations** Bartolomeo Civalleri, L.Donà, J.G.Brandenburg and I.J Bush *University of Torino, Italy*
14:35	Discussion
15:30	Break
	Session 3: Strong correlation in density-functional theory (Session Chair: Paola Gori-Giorgi & Emmanuel Fromager)
16:00	**Embracing local suppression and enhancement of dynamic correlation effects in a CAS-Π-DFT method for efficient description of excited states** Katarzyna Pernal and Oleg V. Gritsenko *Lodz University of Technology, Poland*
16:05	**Multi-state pair-density functional theory** Donald Truhlar, Jie J.Bao, Chen Zhou, Zoltan Varga, Siriluk Kanchanakungwankul and Laura Gagliardi *University of Minnesota, USA*
16:10	Discussion
16:50	Lightning presentations (by invitation of the scientific committee)
17:20	Poster Session
18:20	End of day

Friday 5 September

11:30	**Poster Session**
12:30	**Break**
	Session 4: New approaches to study excited states in density-functional theory (Session Chair: Andrew Teale & Trygve Helgaker)
13:00	**Developing new and understanding old approximations in TDDFT** Neepa Maitra and Lionel Lacombe *Rutgers University at Newark, USA*
13:05	**Weight dependence of local exchange-correlation functionals in ensemble density-functional theory: double excitations in two-electron systems** Pierre-François Loos, Clotilde Marut, Bruno Senjean and Emmanuel Fromager *University of Toulouse, CNRS, France*
13:10	**Design of auxiliary systems for spectroscopy** Matteo Gatti, Marco Vanzini, Francesco Sottile, Igor Reshetnyak, Sergio Ciuchi and

	Lucia Reining *LSI CNRS Ecole Polytechnique, France*
13:15	Discussion
14:15	**Break**
	(Session Chair: Emmanuel Fromager & David Tozer)
14:45	**Variational calculations of excited states via direct optimization of the orbitals in DFT** Gianluca Levi, Aleksei V Ivanov and Hannes Jónsson *University of Iceland, Iceland*
14:50	**Optical spectra of 2D monolayers from time-dependent density functional theory** Pina Romaniello, S. Di Sabatino and J. A Berger *Université de Toulouse, France*
14:55	Discussion
15:35	**Concluding Remarks Lecture** (Session Chair: Andrew Teale) Andreas Savin *CNRS and Sorbonne Université, France*
16:15	**Acknowledgements**
16:30	**Close of meeting**

Please note that timings may change.

Underline indicates the presenting author.