

Symposium Frontiers of Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond (SYES)

jointly organized by
the Surface Science Division (O),
the Metal and Material Physics Division (MM),
the Chemical and Polymer Physics Division (CPP),
the Low Temperature Physics Division (TT),
the Thin Films Division (DS),
the Magnetism Division (MA), and
the Semiconductor Physics Division (HL)

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Density functional theory (DFT) has made an unmatched contribution by providing first-principles atomistic insights to chemistry, condensed matter physics, materials science, and many other fields. However, most commonly used density functional approximations (DFAs) suffer from some well-known failures, including the incapability to correctly describe charge-transfer processes, weak dispersion interactions, and strongly interacting scenarios. Recent effort attempting to cover such intricate many-body effects in DFT has initiated many new concepts at varying theoretical levels, and has led to a bunch of new concepts and insights, as well as new DFAs. Some of these developments can be viewed as a merger of wavefunction theories of quantum chemistry and DFT.

The Symposium “Frontiers of Electronic Structure Theory” is complemented by seven joint sessions hosted by the Surface Science Division (Monday-Thursday). These sessions include four invited talks and more than 70 contributed talks and posters which cover the general field of computational materials science.

Overview of Invited Talks and Sessions

(Lecture room HSZ 02)

Invited Talks

SYES 1.1	Fri	10:30–11:00	HSZ 02	Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — ●WEITAO YANG
SYES 1.2	Fri	11:00–11:30	HSZ 02	Multi-reference density functional theory — ●ANDREAS SAVIN
SYES 1.3	Fri	11:30–12:00	HSZ 02	Density functionals from machine learning — ●KIERON BURKE
SYES 1.4	Fri	12:00–12:30	HSZ 02	Taming Memory-Dependence in Time-Dependent Density Functional Theory — ●NEEPA MAITRA
SYES 1.5	Fri	12:30–13:00	HSZ 02	Quantum Embedding Theories — ●FRED MANBY

Sessions

SYES 1.1–1.5	Fri	10:30–13:00	HSZ 02	Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond
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SYES 1: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Time: Friday 10:30–13:00

Location: HSZ 02

Invited Talk SYES 1.1 Fri 10:30 HSZ 02
Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — ●WEITAO YANG — Duke University

Fractional fractional charges and fractional spins provide a clear analysis of the errors of commonly used functionals. We developed a scaling correction scheme by imposing the Perdew-Parr-Levy-Baldurzi linearity condition. Our novel scheme leads to the significantly improved description of dissociating molecules, transition-state species, and charge-transfer systems. Within many-electron theory, we have formulated the ground-state exchange-correlation energy in terms of pairing matrix linear fluctuations, opening new a channel for density functional approximations. This method has many highly desirable properties. It has minimal delocalization error with a nearly linear energy behavior for systems with fractional charges, describes van der Waals interactions similarly and thermodynamic properties significantly better than the conventional RPA, and captures the energy derivative discontinuity in strongly correlated systems. We also adopted pp-RPA to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct $1/R$ dependence.

Invited Talk SYES 1.2 Fri 11:00 HSZ 02
Multi-reference density functional theory — ●ANDREAS SAVIN — Laboratoire de Chimie Théorique, CNRS and UPMC, Univ. Paris VI, Sorbonne University, Paris, France

It is sometimes said that there is no multi-reference density functional theory. The talk presents a personal viewpoint, and will focus on the following points. 1) There are many ways to introduce multi-determinant wave functions into density functional theory. 2) Several variants have been successfully explored. 3) Difficulties inherent to approximations (both for wave functions and density functionals) persist, but can be attenuated.

Invited Talk SYES 1.3 Fri 11:30 HSZ 02
Density functionals from machine learning — ●KIERON BURKE — UC Irvine

Machine learning is spreading to all aspects of our lives. A particular method, kernel ridge regression, has proven very useful for fitting and interpolating in high-dimensional spaces.

Several years ago, in collaboration with the group of Klaus-Robert Müller in computer science at TU Berlin, we demonstrated how to construct a machine-learned density functional on a simple toy problem, non-interacting fermions in a box. We showed both its successes and limitations. We have continued to develop this method (PRL, 2012).

I will report on two recent works. In the first (arXiv:1609.02815), we construct the non-interacting kinetic energy functional for small molecules in 3D using a basis. We avoid the challenge of finding functional derivatives by learning the potential to density map directly, thereby bypassing the need to solve the Kohn-Sham equations.

In the second, we learn the interacting functional directly for the first time. In 1D, we model chains of H atoms of different length, and learn $F[n]$ itself, from highly accurate DMRG calculations. With a novel choice of basis for the densities, we are able to learn the functional to chemical accuracy in the thermodynamic limit (arXiv:1609.03705).

Invited Talk SYES 1.4 Fri 12:00 HSZ 02
Taming Memory-Dependence in Time-Dependent Density Functional Theory — ●NEEPA MAITRA — Hunter College of the City University of New York

The exact exchange-correlation functional of time-dependent density functional theory (TDDFT) is known to depend on the history of the densities and the initial states, a dependence which is ignored in almost all of the calculations today that use an adiabatic approximation. The lack of this dependence can sometimes lead to drastically incorrect predictions of the dynamics, as has been shown in several examples recently. We present here a new approach to developing functional approximations that breaks free of the adiabatic approximation, and test the resulting approximations on a number of model systems.

Invited Talk SYES 1.5 Fri 12:30 HSZ 02
Quantum Embedding Theories — ●FRED MANBY — School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK

Issues of accuracy in density functional theory can be addressed by making more accurate methods (like coupled-cluster theory) more efficient; or by making density functional approximations more accurate. Efforts in both directions are underway in our group, but in this talk I will focus on a third possibility, namely the development of quantum-mechanical multiscale models that enable the use of a high-accuracy method in a small, physically important region coupled to density-functional theory (or other low-cost methods) to describe the molecular environment.