

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)

John Perdew
Temple University
1925 N. 12th Street
Philadelphia, PA 19122, USA
perdew@temple.edu

Angel Rubio
MPI für Struktur und Dynamik der
Materie
Luruper Chaussee 149
22761 Hamburg
angel.rubio@mpsd.mpg.de

Matthias Scheffler
Fritz-Haber-Institut der MPG
Faradayweg 4-6
14195 Berlin
schefflerfhi-berlin.mpg.de

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
--------------	-----	-------------	--------	--