O 6: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - I

Monday 10:30–13:00 GER 38

Talk O 6.1 Mon 10:30 GER 38
DFT wants U: Embedded-cluster calculations of surface oxygen vacancies at TiO_2 with Hubbard-corrected DFT — •Matthias Kick

Talk O 6.2 Mon 10:45 GER 38
Hubbard interactions from density-functional perturbation theory — •Iurii Timrov

Talk O 6.3 Mon 11:00 GER 38
Time-evolution using full configuration interaction quantum Monte Carlo — •Kai Guther

Talk O 6.4 Mon 11:15 GER 38
Laplace-transformed MP2 with localized Resolution of Identity for molecular and periodic systems — •Arvid Ihrig

Talk O 6.5 Mon 11:30 GER 38
Bond Disproportionation in Rare-Earth Nickelates: Describing Lattice Distortions within DFT+DMFT — •Alexander Hampel

Talk O 6.6 Mon 11:45 GER 38
Density matrix embedding theory for coupled fermion-boson systems — •Teresa E. Reinhard

Talk O 6.7 Mon 12:00 GER 38
Vertex function of homogeneous electron gas — •Yaroslav Pavlyukh

Talk O 6.8 Mon 12:15 GER 38
Coupled-Cluster approaches for molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen

Talk O 6.9 Mon 12:30 GER 38
Implementation of the SU(2) Symmetry in FCIQMC using the Graphical Unitary Group Approach — •Werner Dobrautz

Talk O 6.10 Mon 12:45 GER 38
A study of the dense uniform electron gas with high orders of coupled cluster — •Verena Andrea Neufeld

O 13: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - II

Monday 15:00–18:15 GER 38

Invited Talk O 13.1 Mon 15:00 GER 38
Towards efficient orbital-dependent density functionals for weak and strong correlation — •Igor Ying Zhang

Talk O 13.2 Mon 15:30 GER 38
Towards a functional for strong correlation via semiclassical model for the indirect energy and local interpolation along the adiabatic connection — •Stefan Vuckovic

Talk O 13.3 Mon 15:45 GER 38
Benchmark of *GW* approaches for the *GW*100 test set — •Patrick Rinke

Talk O 13.4 Mon 16:00 GER 38
Addressing electron-hole correlation in core excitations of solids: A first-principles all-electron approach based on many-body perturbation theory — •Christian Vorwerk

Talk O 13.5 Mon 16:15 GER 38
Non-linear-screening contributions to photoemission spectra — •Marilena Tzavala

Talk O 13.6 Mon 16:30 GER 38
Dynamic LDA for electronic excitations — •Marco Vanzini

Talk O 13.7 Mon 16:45 GER 38
Recent developments of the Sternheimer-GW method — •Martin Schlipf

Talk O 13.8 Mon 17:00 GER 38
Calculating electronic correlations in the CASTEP ab initio code — •Vincent Sacksteder

Talk O 13.9 Mon 17:15 GER 38
Efficient G_0W_0 using localized basis sets: a benchmark for molecules — •Peter Koval

Talk O 13.10 Mon 17:30 GER 38
A dynamic exchange correlation kernel derived from recent results for the homogeneous electron gas — •Martin Panholzer

Talk O 13.11 Mon 17:45 GER 38
Benchmark calculations of the electronic structure for molecules from the second-Born self-energy — •Michael Schüler

Talk O 13.12 Mon 18:00 GER 38
Performance of the GW approximation at reproducing key features in exact Kohn-Sham potentials — •Jack Wetherell

O 30: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - III

Tuesday 10:30–13:00 GER 38

Invited Talk O 30.1 Tue 10:30 GER 38
Including spin effects in the strong-coupling limit of DFT — •Paola Gori-Giorgi

Talk O 30.2 Tue 11:00 GER 38
Strong correlation from the Random Phase Approximation and beyond — •Thomas Olsen

Talk O 30.3 Tue 11:15 GER 38
Surface and adsorption energy calculations within the random phase approximation — •Per Schmidt

Talk O 30.4 Tue 11:30 GER 38
Large-scale cubic-scaling RPA correlation energy calculations using a Gaussian basis — •Jan Wilhelm

Talk O 30.5 Tue 11:45 GER 38
Semi-local exchange functionals showing ultranonlocal re-

sponse: the hope to replace exact exchange — •Thilo Aschebrock

Talk O 30.6 Tue 12:00 GER 38
(De)stabilizing dispersion interactions via external electric charges — •Andrii Kleshchonok

Talk O 30.7 Tue 12:15 GER 38
An optimisability proof for self-consistent constrained DFT, and its implications for constraint-based self-interaction error correction — •David D. O'Regan

Talk O 30.8 Tue 12:30 GER 38
Density-based local hybrid functional for interfaces — •Pedro Borlido

Talk O 30.9 Tue 12:45 GER 38
On the hunt for better functionals in DFT: a new quantum embedding scheme — •Uliana Mordovina

O 65: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Tuesday 18:30–20:30 P2-OG4

Poster O 65.1 Tue 18:30 P2-OG4
Angular projection potentials for density functional calculations — •Rudolf Zeller

Poster O 65.2 Tue 18:30 P2-OG4
DFPT within the All-Electron FLAPW Method: Application to Phonons — •Christian-Roman Gerhorst

Poster O 65.3 Tue 18:30 P2-OG4
Conceptual problemsof self-interaction corrections — •Charlotte Vogelbusch

Poster O 65.4 Tue 18:30 P2-OG4
Numerical improvements of Fermi-Löwdin orbital self-interaction correction — •Lenz Fiedler

Poster O 65.5 Tue 18:30 P2-OG4
Electronic and Magnetism Properties of Vacancy-Defected, Fluorine Doped and Adsorption upon MO3 (M= Cr, Mo, W) Surface: a first-principles study — •Masoud Mansouri

Poster O 65.6 Tue 18:30 P2-OG4
An Investigation of Group V dopants in Silicon using Linear Scaling DFT — •Jack Poulton

Poster O 65.7 Tue 18:30 P2-OG4
Deciphering chemical bonding with Fermi-Löwdin orbitals — •Torsten Hahn

Poster O 65.8 Tue 18:30 P2-OG4
Binding energy curves for diatomic molecules obtained by FLO-SIC DFT — •Simon Liebing

Poster O 65.9 Tue 18:30 P2-OG4
Groundstates of the ternary clathrate $Ba_8Ni_xGe_{46-x-y}\square_y$ obtained with an iterative cluster expansion approach — •Martin Kuban

Poster O 65.10 Tue 18:30 P2-OG4
The inapplicability of exact constraints, and a minimal two-parameter DFT+U generalisation, for self-interaction error correction — •Glenn Moynihan

Poster O 65.11 Tue 18:30 P2-OG4
A Hubbard U based correction method for exciton binding in neutral excitations: TDDFT+U — •Okan K. Orhan

Poster O 65.12 Tue 18:30 P2-OG4
Implementation of Electron-Phonon Coupling in the KKR Formalism and its Applications to Simple Metals — •Michael Czerner

O 71: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - IV

Wednesday 10:30–13:00 GER 38

Invited Talk O 71.1 Wed 10:30 GER 38
Electronic excitations in 2D materials and heterostructures — •Kristian Sommer Thygesen

Talk O 71.2 Wed 11:00 GER 38
Charge and energy transport at the nanoscale: A DFT perspective — •Florian G. Eich

Talk O 71.3 Wed 11:15 GER 38
Conductance of aromatic and antiaromatic molecular circuits — •Héctor Vázquez

Talk O 71.4 Wed 11:30 GER 38
Current-induced cooling of Carbene-based molecular junctions: role of electrodes structure — •Giuseppe Foti

Talk O 71.5 Wed 11:45 GER 38
DFTB-based recursive Green's function algorithms for electron transport in quasi-1D systems — •Fabian Teichert

Talk O 71.6 Wed 12:00 GER 38
Conditions for formation of two-dimensional electron gas at the $LaFeO_3/SrTiO_3$ — •Igor Maznichenko

Talk O 71.7 Wed 12:15 GER 38
Thermal Renormalization of the Electronic Structure: Trends across Chemical and Structural Space — •Honghui Shang

Talk O 71.8 Wed 12:30 GER 38
Spin-wave excitations and electron-magnon scattering from many-body perturbation theory — •Mathias C.T.D. Müller

Talk O 71.9 Wed 12:45 GER 38
Charged supercells revised: Small Polarons in Oxides with proper account for long-range polarization — •Sebastian Kokott

O 78: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - V

Wednesday 15:00–18:15 GER 38

Talk O 78.1 Wed 15:00 GER 38
First-principle Linear Response in Real Space — •Honghui Shang

Talk O 78.2 Wed 15:15 GER 38
Anharmonic Vibrations in Solids: Why and When Going Beyond Perturbative Treatments is Necessary — •Hagen-Henrik Kowalski

Talk O 78.3 Wed 15:30 GER 38
Anharmonic and Quantum Fluctuations in Molecular Crystals from Ab Initio Simulations — •Mariana Rossi

Talk O 78.4 Wed 15:45 GER 38
Exact solutions and approximations in the exact factorization of the electron-nuclear wavefunction — •Graeme Gossel

Talk O 78.5 Wed 16:00 GER 38
Insight into time-propagation TDDFT excitations via Kohn–Sham decomposition — •Tuomas P. Rossi

Talk O 78.6 Wed 16:15 GER 38
Gauge-invariant Magnetic Properties from Time-Dependent Current-Density-Functional Theory — •Nathaniel Raimbault

Talk O 78.7 Wed 16:30 GER 38
Calculation of charge transfer integrals using constrained-DFT — •Tobias Lettmann

Talk O 78.8 Wed 16:45 GER 38
Towards ultra long-range ab-initio calculations — •Tristan Müller

Talk O 78.9 Wed 17:00 GER 38
Local density fitting within a Gaussian and plane waves scheme for large-scale density functional theory calculations — •Dorothea Golze

Talk O 78.10 Wed 17:15 GER 38
From the Electron Localization Function to a Coalescent-Pair Locator — •Stefano Pittalis

Talk O 78.11 Wed 17:30 GER 38
Band structure interpolation via maximally localized Wannier functions implemented in LAPW+lo basis — •Sebastian Tillack

Talk O 78.12 Wed 17:45 GER 38
Chemical insight from Fermi-Löwdin orbitals — •Torsten Hahn

Talk O 78.13 Wed 18:00 GER 38
Conditions for describing triplet states in reduced density matrix functional theory — •Nicole Helbig

O 88: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VI

Thursday 10:30–13:45 GER 38

Talk O 88.1 Thu 10:30 GER 38
Implicit solvation functionality in FHI-aims: Kirkwood multipole expansion model — •Markus Sinstein

Talk O 88.2 Thu 10:45 GER 38
Using Dipsersion-Corrected Density Functional Theory to Understand the Phase Diagram of Alkanethiolates on Gold — •Joakim Löfgren

Talk O 88.3 Thu 11:00 GER 38
Finite-temperature properties of the thermoelectric clathrate $Ba_8Al_xSi_{46-x}$ — •Maria Troppenz

Talk O 88.4 Thu 11:15 GER 38
Electronic structure and solid-state optical properties of indigo from time-dependent optimally tuned range-separated hybrid functional theory — •Bernd Kollmann

Talk O 88.5 Thu 11:30 GER 38
Thermodynamic properties from ab-initio calculations - Ti as a case study — •Guy Makov

Talk O 88.6 Thu 11:45 GER 38
Molecular orbitals in the bismuth perovskites — •Kateryna Foyevtsova

Talk O 88.7 Thu 12:00 GER 38
Ab initio calculations and strain-dependent scaling of excitons in carbon nanotubes — •Christian Wagner

Talk O 88.8 Thu 12:15 GER 38
Dzyaloshinskii-Moriya-interaction energy, where it is located? Real and reciprocal spaces views. — •Leonid Sandratskii

Talk O 88.9 Thu 12:30 GER 38
***Ab-initio* study of the Raman spectra of strained graphene** — •Albin Hertrich

Talk O 88.10 Thu 12:45 GER 38
DFT meets Landau Theory: The High Pressure Phase Transition of Lead Titanate — •Andreas Tröster

Talk O 88.11 Thu 13:00 GER 38
Ground-State and Excitation Properties of Orthorhombic $MAPbI_3$ — •Claudia Rödl

Talk O 88.12 Thu 13:15 GER 38
Structure, nonstoichiometry, and geometrical frustration of α-tetragonal boron — •Jens Kunstmann

Talk O 88.13 Thu 13:30 GER 38
Magnetic response properties of thin films using Kubo's linear response formalism — •Andreas Held

O 99: Electronic Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond - VII

Thursday 16:00–18:30 GER 38

Invited Talk O 99.1 Thu 16:00 GER 38
Spectacular success of DFT in predicting novel topological phases — •Arun Bansil

Talk O 99.2 Thu 16:30 GER 38
Interlayer excitons and Band Alignment in MoS_2/hBN/WSe_2 van der Waals Heterostructures — •Simone Latini

Talk O 99.3 Thu 16:45 GER 38
Trionic effects in graphene nanoribbons and further nanomaterials — •Thorsten Deilmann

Talk O 99.4 Thu 17:00 GER 38
Interface Structure Prediction using the Ab Initio Random Structure Searching Method — •Georg Schusteritsch

Talk O 99.5 Thu 17:15 GER 38
Predicting new materials and their properties with supercomputers: the example of perovskites — •Silvana Botti

Talk O 99.6 Thu 17:30 GER 38
Spectral property prediction with artificial neural networks — •Annika Stuke

Talk O 99.7 Thu 17:45 GER 38
Machine-Learning Based Interatomic Potential for Amorphous Carbon — •Volker Deringer

Talk O 99.8 Thu 18:00 GER 38
High-throughput computational search for new high mobility transparent (semi)conducting materials — •Geoffroy Hautier

Talk O 99.9 Thu 18:15 GER 38
Cross-validation in the cluster expansion method — •Axel Hübner

SYES 1: Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond

Friday 10:30–13:00 HSZ 02

Invited Talk SYES 1.1 Fri 10:30 HSZ 02
Going Beyond Conventional Functionals with Scaling Corrections and Pairing Fluctuations — •Weitao Yang

Invited Talk SYES 1.2 Fri 11:00 HSZ 02
Multi-reference density functional theory — •Andreas Savin

Invited Talk SYES 1.3 Fri 11:30 HSZ 02
Density functionals from machine learning — •Kieron Burke

Invited Talk SYES 1.4 Fri 12:00 HSZ 02
Taming Memory-Dependence in Time-Dependent Density Functional Theory — •Neepa Maitra

Invited Talk SYES 1.5 Fri 12:30 HSZ 02
Quantum Embedding Theories — •Fred Manby