O 19: Frontiers of Electronic Structure Theory: Many-Body Effects on the Nano-Scale I

Tuesday 10:30–13:30 MA 004

Invited Talk O 19.1 Tue 10:30 MA 004
Electronic structure in the vicinity of strong non-adiabatic couplings — •Eberhard K.U. Gross

Talk O 19.2 Tue 11:00 MA 004
Towards First-Principles Modeling of Electrolytic Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe

Talk O 19.3 Tue 11:15 MA 004
Phonons in Molecular Crystals: The Role of Collective van der Waals Interactions — •Johannes Hoja

Talk O 19.4 Tue 11:30 MA 004
Converged Nuclear Quantum Statistics from Semi-Classical Path Integrals — •Igor Poltavskyi

Talk O 19.5 Tue 11:45 MA 004
Can we get reliable quantum dynamics simulations for vibrational spectra in the condensed phase? — •Mariana Rossi

Talk O 19.6 Tue 12:00 MA 004
Ultra-high temperature properties of ZrC: a fully-anharmonic ab-initio approach — •Andrew Duff

Talk O 19.7 Tue 12:15 MA 004
Quo vadis electronic friction? Assessing vibrational lifetimes beyond the independent atom approximation — •Simon P. Rittmeyer

Talk O 19.8 Tue 12:30 MA 004
Polynomial-oriented linear least squares fits of potential energy surfaces for quantum dynamics — •Florian Habecker

Talk O 19.9 Tue 12:45 MA 004
Representing Complex Potential Energy Surfaces by Artificial Neural Networks — •Christopher Handley

Talk O 19.10 Tue 13:00 MA 004
Kinetic Monte Carlo simulations of thin film growth with anisotropic particles — •Miriam Klopotek

Talk O 19.11 Tue 13:15 MA 004
Ti and N adatom diffusion on, and N_2 desorption from TiN(001) surfaces via *ab initio* and classical molecular dynamics — •Davide G. Sangiovanni

O 26: Frontiers of Electronic Structure Theory: Many-Body Effects on the Nano-Scale II

Tuesday 14:00–15:45 MA 004

Invited Talk O 26.1 Tue 14:00 MA 004
First-principles theories of electron-plasmon and electron-spin fluctuation interactions in nanomaterials — •Johannes Lischner

Talk O 26.2 Tue 14:30 MA 004
Charge separation dynamics and opto-electronic properties of a diaminoterephthalate-C60 dyad — •Stefano Pittalis

Talk O 26.3 Tue 14:45 MA 004
Transfering spin into an extended π-orbital of a large molecule – ab-initio study of Au-PTCDA:Au(111) — •T. Deilmann

Talk O 26.4 Tue 15:00 MA 004
Quasi-particle band structure of the transition-metal-based zero-gap semiconductors — •Murat Tas

Talk O 26.5 Tue 15:15 MA 004
Keldysh nonequilibrium Green's function vs. Feshbach projection operator approach for plasmon-assisted photoemission — •Yaroslav Pavlyukh

Talk O 26.6 Tue 15:30 MA 004
Inclusion of thermal lattice vibrations and spin fluctuations within transport calculations — •Sergiy Mankovsky

O 47: Frontiers of Electronic Structure Theory: Many-Body Effects on the Nano-Scale III

Wednesday 10:30–13:30 MA 004

Invited Talk O 47.1 Wed 10:30 MA 004
Transport and excitations in biased nano-junctions: DFT-based simulations — •Mads Brandbyge

Talk O 47.2 Wed 11:00 MA 004
Role of atomic multiplets in intermediate valence SmB_6 and PuB_6 systems — •Alexander B. Shick

Talk O 47.3 Wed 11:15 MA 004
Transition paths and cohesive energies in alpha-sexithiophene polymorphs — •Bernhard Klett

Talk O 47.4 Wed 11:30 MA 004
Importance of the reorganization energy barrier in computational design of porphyrin-based solar cells with cobalt-based redox mediators — •Kristian Baruël Ørnsø

Talk O 47.5 Wed 11:45 MA 004
Ab initio Simulation of Optical Limiting: The Case of Metal-Free Phthalocyanine — •Caterina Cocchi

Talk O 47.6 Wed 12:00 MA 004
High-throughput Screening of Perovskite Oxides and Related Compounds for Light Harvesting Applications — •Ivano E. Castelli

Talk O 47.7 Wed 12:15 MA 004
Understanding and designing novel materials for energy — •Silvana Botti

Talk O 47.8 Wed 12:30 MA 004
Accurate density-functional theory calculation of bulk properties of 65 elemental solids — •Sven Lubeck

Talk O 47.9 Wed 12:45 MA 004
Electronic phase transitions of bismuth under strain from relativistic self-consistent *GW* calculations — •Christoph Friedrich

Talk O 47.10 Wed 13:00 MA 004
A GW algorithm of reduced complexity for organic crystals — •Saber Gueddida

Talk O 47.11 Wed 13:15 MA 004
Modeling anisotropic organic molecules at patterned semiconductor surfaces — •Nicola Kleppmann

O 56: Frontiers of Electronic Structure Theory: Many-Body Effects on the Nano-Scale IV

Wednesday 15:00–18:30 MA 004

Invited Talk O 56.1 Wed 15:00 MA 004
Ultrafast coherent dynamics in photovoltaics — •Carlo Andrea Rozzi

Talk O 56.2 Wed 15:30 MA 004
Real-time propagation of coupled Maxwell-Kohn-Sham systems — •Rene Jestädt

Talk O 56.3 Wed 15:45 MA 004
Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick

Talk O 56.4 Wed 16:00 MA 004
A hybrid QM/EMT approach to charge state corrections — •Osman Baris Malcioglu

Talk O 56.5 Wed 16:15 MA 004
Plasmon assisted double photoemission — •Michael Schüler

Talk O 56.6 Wed 16:30 MA 004
Calculating photoemission spectra with real-time density-functional theory — •Matthias Dauth

Talk O 56.7 Wed 16:45 MA 004
***Ab initio* local field effects for surface second harmonic generation** — •Nicolas Tancogne-Dejean

Talk O 56.8 Wed 17:00 MA 004
Mapping atomic orbitals in the transmission electron microscope: seeing defects in graphene — •Lorenzo Pardini

Talk O 56.9 Wed 17:15 MA 004
Inelastic X-Ray Scattering: Insights from and Benefits for Many-Body Theory — •Claudia Rödl

Talk O 56.10 Wed 17:30 MA 004
Real-Space Multiple-Scattering X-ray Absorption Spectroscopy Calculations of d- and f-state Materials using a Hubbard Model — •Christian Vorwerk

Talk O 56.11 Wed 17:45 MA 004
Variants of Second Order Screened Exchange for spin polarized and non-polarized Uniform Electron Gas — •Felix Hummel

Talk O 56.12 Wed 18:00 MA 004
Ferromagnetism from strongly correlated electrons at the $LaAlO_3/SrTiO_3$ interface — •Frank Lechermann

Talk O 56.13 Wed 18:15 MA 004
NanoDMFT: Full ab initio description of strong correlations in nanoscale devices — •David Jacob

O 78: Frontiers of Electronic Structure Theory: Many-Body Effects on the Nano-Scale V

Thursday 10:30–13:15 MA 004

Invited Talk O 78.1 Thu 10:30 MA 004
Interaction and Correlation Effects in Quasi Two-dimensional Materials — •Steven G. Louie

Talk O 78.2 Thu 11:00 MA 004
Screening of the Coulomb interaction in two-dimensional semiconductors: The case of transition metal dichalcogenides — •Ersoy Sasioglu

Talk O 78.3 Thu 11:15 MA 004
Ultra-fast transient absorption spectra of monolayer MoS2 by first principle — •Margherita Marsili

Talk O 78.4 Thu 11:30 MA 004
Plasmon and exciton dispersion in two dimensions — •Pier Luigi Cudazzo

Talk O 78.5 Thu 11:45 MA 004
Origin of metallic edge states in transition-metal-dichalcogenide nanostructures — •Marco Gibertini

Talk O 78.6 Thu 12:00 MA 004
Starting-point dependence in the Bethe-Salpeter equation: example of rutile TiO_2 — •Olga Turkina

Talk O 78.7 Thu 12:15 MA 004
Efficient exchange-correlation kernels for the description of excitonic effects in solids — •Santiago Rigamonti

Talk O 78.8 Thu 12:30 MA 004
Excitonic effects in many-body calculations — •Matteo Gatti

Talk O 78.9 Thu 12:45 MA 004
Efficient parameter-free calculation of absorption spectra for insulators, semiconductors and metals from time-dependent current DFT — •Arjan Berger

Talk O 78.10 Thu 13:00 MA 004
Optical excitations in MoS_2 within ab-initio many-body perturbation theory — •Matthias Drüppel

O 85: Frontiers of Electronic Structure Theory: Many-Body Effects on the Nano-Scale VI

Thursday 15:00–18:30 MA 004

Invited Talk O 85.1 Thu 15:00 MA 004
Natural orbital functional theory with higher-order occupation probabilities — •Ralph Gebauer

Talk O 85.2 Thu 15:30 MA 004
Electronic Properties of Surfaces and Interfaces with Self-Consistent Interatomic van der Waals Density Functional — •Nicola Ferri

Talk O 85.3 Thu 15:45 MA 004
Exact functionals for a lattice model — •Tanja Dimitrov

Talk O 85.4 Thu 16:00 MA 004
Many-body dispersion meets non-local density functionals: A unified approach for van der Waals correlations — •Jan Hermann

Talk O 85.5 Thu 16:15 MA 004
Reduced Density-Matrix Functional Theory: correlation and spectroscopy — •Pina Romaniello

Talk O 85.6 Thu 16:30 MA 004
Does GW obey the straight-line condition? — •Patrick Rinke

Talk O 85.7 Thu 16:45 MA 004
Green's Function embedding for Advanced Electronic Structure Methods based on Dynamical Mean-Field Theory — •Wael Chibani

Talk O 85.8 Thu 17:00 MA 004

Improved Ground State Electronic Structure and Optical Dielectric Constants With a Semi-Local Exchange Functional — •Vojtěch Vlček

Talk O 85.9 Thu 17:15 MA 004
Accurate, efficient localized resolution of identity of the Coulomb operator across the periodic table — •Arvid Ihrig

Talk O 85.10 Thu 17:30 MA 004
Explicitly correlated self consistent field theory — •Christian Lasar

Talk O 85.11 Thu 17:45 MA 004
Comparison of two self-consistent *GW* schemes — •Peter Koval

Talk O 85.12 Thu 18:00 MA 004
Quasiparticle Self-Consistent *GW* for Molecules — •Ferdnand Kaplan

Talk O 85.13 Thu 18:15 MA 004
Pure state N-representability conditions: Should they be taken into account in Reduced density matrix functional theory? — •Iris Theophilou

O 94: Frontiers of Electronic Structure Theory: Many-body Effects on the Nano-scale

Friday 09:30–12:15 H 0105

Invited Talk O 94.1 Fri 9:30 H 0105
Excitations and charge transfer phenomena in C based systems — •Elisa Molinari

Invited Talk O 94.2 Fri 10:00 H 0105
Towards optimal correlation factors for many-electron perturbation theories — •Andreas Grüneis

Invited Talk O 94.3 Fri 10:30 H 0105
Towards an ab-initio description of high temperature superconductivity — •Garnet Chan

Coffee break

Invited Talk O 94.4 Fri 11:15 H 0105
Correlation effects in unconventional superconductors: from micro- to nano- and macroscales. — •Roser Valenti

Invited Talk O 94.5 Fri 11:45 H 0105
Stochastic density functional and GW theories scaling linearly with system size — •Roi Baer