Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale

Monday 10:30–13:15 TRE Ma

Topical Talk O 7.1 Mon 10:30 TRE Ma
Molecular junction transport: some theoretical and computational considerations — •Mark Ratner[1] and Matthew Reuter[2] — [1]Chemistry, Northwestern University, Evanston Illinois 60208 USA — [2]Chemistry, Northwestern University, Evanston Illinois 60208 USA

Talk O 7.2 Mon 11:00 TRE Ma
On the description of biased nanocontacts from ab initio — •Steven Achilles[1], Jürgen Henk[1], Michael Czerner[2], Christian Heiliger[2], and Ingrid Mertig[1] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany — [2]I. Physikalisches Institut, Justus Liebig University, D-35392 Giessen, Germany

Talk O 7.3 Mon 11:15 TRE Ma
Elasticity changes in molecular junctions under bias: an ab-initio study — •Clotilde S. Cucinotta[1], Meilin Bai[1,2], Ivan Rungger[1], Shmin Hou[2], and Stefano Sanvito[1] — [1]School of Physics and CRANN, Trinity College Dublin, College Green, Dublin 2, Ireland — [2]2Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Talk O 7.4 Mon 11:30 TRE Ma
Carbon nanotubes decorated with magnetic clusters: magnetism, electron transport and gas sensing — •Zeila Zanolli[1] and Jean-Christophe Charlier[2] — [1]Forschungszentrum Juelich, PGI and IAS, Juelich, Germany — [2]IMCN, Université catholique de Louvain (UCL), Belgium

15 min. break

Topical Talk O 7.5 Mon 12:00 TRE Ma
Insight into Charge Transport in Molecular Junctions from Ab Initio Theories of Level Alignment — •Jeffrey B. Neaton — Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA — Department of Physics, University of California, Berkeley, Berkeley, CA — Kavli Energy Nanosciences Institute, Berkeley, CA

Talk O 7.6 Mon 12:30 TRE Ma
Towards First-Principles Modeling of Solvent Effects in Photo-Catalytic Water Splitting — •Stefan Ringe, Harald Oberhofer, Sebastian Matera, and Karsten Reuter — Technische Universität München, Germany

Talk O 7.7 Mon 12:45 TRE Ma
Towards a combined QM/MM and implicit solvent description of photoelectrochemical processes — •Markus Sinstein[1], Daniel Berger[1], Ran Jia[2], Volker Blum[3], Harald Oberhofer[1], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Jilin University, P.R. China — [3]Duke University, USA

Talk O 7.8 Mon 13:00 TRE Ma
Ab-initio Simulation of Molecular Networks on the Surface of Water — •Ralph Koitz, Marcella Iannuzzi, Ari P Seitsonen, and Jürg Hutter — University of Zurich, Zurich, Switzerland

Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale II

Monday 16:00–18:45 TRE Ma

Topical Talk O 15.1 Mon 16:00 TRE Ma
Simulating heat transport: from large scale molecular dynamics to first-principles calculations — •Davide Donadio — Max Planck Institute for Polymer Research, Mainz, Germany

Talk O 15.2 Mon 16:30 TRE Ma
First principles study of thermal conductivity cross-over in nano-structured Zinc-Chalcogenides — •Ankita Katre[1], Atsushi Togo[2], Ralf Drautz[1], and Georg K. H. Madsen[1] — [1]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]ESISM, Kyoto University, Sakyo, Kyoto 606-8501, Japan

Talk O 15.3 Mon 16:45 TRE Ma
Density-functional perturbation theory for lattice dynamics with numeric atom-centered orbitals — •Honghui Shang, Christian Carbogno, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin

Talk O 15.4 Mon 17:00 TRE Ma
Breakdown of Fourier law in layered materials — •Andrea Cepellotti[1], Giorgia Fugallo[2], Francesco Mauri[3], and Nicola Marzari[1] — [1]THEOS, École Polytechnique Fédérale, Lausanne — [2]IMPMC, Universite Pierre et Marie Curie, Paris — [3]LSI, École Polytechnique, Paris

Talk O 15.5 Mon 17:15 TRE Ma
High Temperature Thermal Conductivity from First Principles — •Christian Carbogno[1], Rampi Ramprasad[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Chemical, Materials & Biomolecular Engineering, University of Connecticut, Storrs, USA

Talk O 15.6 Mon 17:30 TRE Ma
Accurate Modelling of the Polymorphism and Elastic Response of Molecular Materials from First Principles — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Talk O 15.7 Mon 17:45 TRE Ma
Surface chemistry on nanostructured oxides: do we have to go beyond hybrid DFT? — •Daniel Berger, Harald Oberhofer, and Karsten Reuter — Technische Universität München, Germany

Talk O 15.8 Mon 18:00 TRE Ma
Atoms-in-solids perspective on polarizabilities and van der Waals coefficients in semiconductors — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

Talk O 15.9 Mon 18:15 TRE Ma
Adsorption at semiconductor surfaces - an energy analysis method — •Ralf Tonner and Marc Raupach — Fachbereich Chemie & Materials Sciences Centre, Philipps-Universität Marburg, Germany

Talk O 15.10 Mon 18:30 TRE Ma
Non-local density functionals meet many-body dispersion: A hybrid approach for van der Waals interactions — •Jan Hermann, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale III

Tuesday 10:30–13:15 TRE Ma

Topical Talk O 28.1 Tue 10:30 TRE Ma
Ultrafast relaxation dynamics of Hubbard nanoclusters — •Michael Bonitz[1], Sebastian Hermanns[1], Christopher Hinz[1], and Denis Lacroix[2] — [1]Institut für Theoretische Physik und Astrophysk, CAU Kiel, Leibnizstr. 15, 24098 Kiel — [2]IPN Orsay, 15 Rue Georges Clemenceau, 91406 Orsay

Talk O 28.2 Tue 11:00 TRE Ma
Exact adiabatic approximation in TDDFT — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Talk O 28.3 Tue 11:15 TRE Ma
Real-time propagation of coupled Maxwell-Schrödinger and time-dependent Kohn-Sham-Maxwell systems — •René Jestädt[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Talk O 28.4 Tue 11:30 TRE Ma
Nonlinear optics by means of the dynamical Berry phase: Application to second- and third-harmonic generation — •Claudio Attaccalite[1] and Myrta Gruning[2] — [1]Univ. Grenoble Alpes/CNRS, Institut Neel, F-38042 Grenoble, France — [2]School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK

15 min. break

Talk O 28.5 Tue 12:00 TRE Ma
Accurate Correlation Energies from Adiabatic Time-Dependent Density Functional Theory with Renormalized Kernels — •Thomas Olsen[1] and Kristian S. Thygesen[2] — [1]Universidad del Pais Vasco — [2]Center for Atomic-scale Materials Design (CAMD), Technical University of Denmark

Talk O 28.6 Tue 12:15 TRE Ma
Low scaling algorithm for the random phase approximation — •Merzuk Kaltak, Jiri Klimeš, and Georg Kresse — University of Vienna, Computational Material Physics

Talk O 28.7 Tue 12:30 TRE Ma
Long range correlation energy from coupled atomic response functions — •Alberto Ambrosetti and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Faradayweg 4-6 14195 Berlin, Germany

Talk O 28.8 Tue 12:45 TRE Ma
The exact Hohenberg-Kohn functional for a lattice model — •Tanja Dimitrov[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Talk O 28.9 Tue 13:00 TRE Ma
Incorporating static correlation effects into density functional theory — Nektarios N. Lathiotakis[1], •Nicole Helbig[2], Nikitas I. Gidopoulos[3], and Angel Rubio[4,5] — [1]Theoretical and Physical Chemistry Institute, NHRF Athens, Greece — [2]Peter-Grünberg Institut, Forschungszentrum Jülich, Germany — [3]Department of Physics, Durham University, United Kingdom — [4]Nano-Bio Spectroscopy group, Universidad del Pais Vasco and DIPC, San Sebastian, Spain — [5]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale IV

Wednesday 10:30–13:15 TRE Ma

Topical Talk O 47.1 Wed 10:30 TRE Ma
From Rydberg Crystals to Bound Magnons - Probing the Non-Equilibrium Dynamics of Ultracold Atoms in Optical Lattices — •Immanuel Bloch — Max-Planck Institut für Quantenoptik, Garching, Germany — Ludwig-Maximilians-Universität, Munich, Germany

Talk O 47.2 Wed 11:00 TRE Ma
Correlated Light-Matter Interactions in Cavity QED — •Johannes Flick[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Talk O 47.3 Wed 11:15 TRE Ma
Optimized effective potential approach to time-dependent density functional theory for many-electron systems interacting with cavity photons — •Camilla Pellegrini[1], Johannes Flick[2], Heiko Appel[2], Ilya V. Tokatly[1,3], and Angel Rubio[1,2] — [1]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Física de Materiales, Universidad del País Vasco UPV/EHU, E-20018 San Sebastían, Spain — [2]Fritz-Haber Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [3]IKERBASQUE, Bilbao, Spain

Talk O 47.4 Wed 11:30 TRE Ma
Correlated photon-electron wavefunctions in cavity Quantum Electrodynamics — •Heiko Appel[1], Johannes Flick[1], Rene Jestaedt[1], and Angel Rubio[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Talk O 47.5 Wed 11:45 TRE Ma
Photoelectron driven plasmaron excitations in (2x2)K/Graphite — •Bo Hellsing — Department of Physics, Gothenburg University, Sweden

Talk O 47.6 Wed 12:00 TRE Ma
Charge-transfer excitations in organic systems from many-body perturbation theory — •Xavier Blase[1], Carina Faber[1,2], Paul Boulanger[1], Claudio Attaccalite[1], and Ivan Duchemin[2] — [1]Institut Néel, CNRS and UJF, Grenoble, France — [2]L_SIM/INAC, CEA, Grenoble, France

Talk O 47.7 Wed 12:15 TRE Ma
Charge transfer from first principles: self-consistent *GW* applied to donor-acceptor systems — •Fabio Caruso[1,2], Viktor Atalla[1], Angel Rubio[1,3], Matthias Scheffler[1], and Patrick Rinke[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Oxford, UK — [3]Universidad del País Vasco, San Sebastián, Spain

Talk O 47.8 Wed 12:30 TRE Ma
What Koopmans' compliant orbital-density dependent functionals can do for you: a comprehensive benchmark of the G2-set — •Giovanni Borghi[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]École Polytechnique Fédérale de Lausanne, Lausanne (VD), CH — [2]Centro S3, CNR–NANO, Modena, IT — [3]Department of Materials Science and Engineering, Penn State University, University Park (PA), USA

Talk O 47.9 Wed 12:45 TRE Ma
The electronic structure of quinacridone: Optimally tuned range-separated hybrid functional versus GW results — Daniel Lüftner[1], Sivan Refaely-Abramson[2], Michael Pachler[1], Michael G. Ramsey[1], Leeor Kronik[2], and •Peter Puschnig[1] — [1]Institut für Physik, Karl-Franzens-Universität Graz, Austria —

[2]Department of Materials and Interfaces, Weizmann Institute of Science, Israel

Talk O 47.10 Wed 13:00 TRE Ma

GW many-body perturbation theory for electron-phonon coupling calculations — •Carina Faber[1,2], Paul Boulanger[1], Ivan Duchemin[1,2], and Xavier Blase[1] — [1]Institut Néel, CNRS, Grenoble, France — [2]INAC, CEA, Grenoble, France

Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale V

Wednesday 16:00–19:15 TRE Ma

Topical Talk O 56.1 Wed 16:00 TRE Ma
Theory of nonlinear phononics for coherent light-control of solids — •Antoine Georges[1,2,3], Alaska Subedi[2], and Andrea Cavalleri[4] — [1]College de France, Paris, France — [2]Ecole Polytechnique - CPHT, Palaiseau, France — [3]University of Geneva, DPMC, Switzerland — [4]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Talk O 56.2 Wed 16:30 TRE Ma
DFT+Frontier Orbital U — •Emine Kucukbenli and Nicola Marzari — Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH)

Talk O 56.3 Wed 16:45 TRE Ma
Quasiparticle self-consistent *GW* method with spin-orbit coupling applied to Bi and HgTe — •Christoph Friedrich, Irene Aguilera, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Talk O 56.4 Wed 17:00 TRE Ma
Studies of semiconducting pyrite and marcasite compounds using many-body perturbation theory in the *GW* approximation — •Timo Schena, Gustav Bihlmayer, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Germany

15 min. break

Talk O 56.5 Wed 17:30 TRE Ma
Probing d-band Quantum Well States in Palladium Nanofilms — •Srijan Kumar Saha[1], Sujit Manna[1], Marek Przybylski[1,2], Valeri Stepanyuk[1], and Jurgen Kirschener[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, 30-059 Kraków, Poland — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Talk O 56.6 Wed 17:45 TRE Ma
Implementation and analysis of a plane wave and real space pseudopotential method including an efficient spin-orbit coupling treatment tailored to calculate the electronic structure of large-scale semiconductor nanostructures — •Frank Zirkelbach, Pierre-Yves Prodhomme, Jerome Jackson, and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany

Talk O 56.7 Wed 18:00 TRE Ma
Strong Parallelization of Real-Space DFT Calculations — •Andrea Nobile[1,2], Paul Baumeister[1,2], Daniel Wortmann[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungzentrum Jülich and JARA, 52425 Jülich, Germany — [2]Jülich Supercomputing Center, Forschungzentrum Jülich, 52425 Jülich, Germany

Talk O 56.8 Wed 18:15 TRE Ma
Rare Earth Metals in Density-Functional Theory — •Marco Casadei[1], Xinguo Ren[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Technology, Hefei, China — [3]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain

Talk O 56.9 Wed 18:30 TRE Ma
Electronic Structure and van der Waals Interactions in the Stability and Mobility of Point Defects in Semiconductors — •Wang Gao and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Talk O 56.10 Wed 18:45 TRE Ma
Scaling Laws for van der Waals Interactions in Nanostructured Materials — •Vivekanand Gobre and Alexandre Tkatchenko — Fritz Haber Institut der MPG, Berlin

Talk O 56.11 Wed 19:00 TRE Ma
2D nanopatterns of shape-persistent molecular polygons on HOPG — •Stefan-S. Jester, Nina Schönfelder, Eva Sigmund, and Sigurd Höger — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Focussed Session: Frontiers of Electronic Structure Theory - Non-equilibrium Phenomena at the Nano-scale VI

Thursday 10:30–13:15 TRE Ma

Topical Talk O 70.1 Thu 10:30 TRE Ma
Localization at the edge of 2D topological insulator by Kondo impurities — •Boris Altshuler[1], Igor Aleiner[1], and Vladimir Yudson[2] — [1]Physics Department, Columbia University, New York, NY 10027, USA — [2]Institute for Spectroscopy, Russian Academy of Sciences,Troitsk, Moscow 142190, Russia

Talk O 70.2 Thu 11:00 TRE Ma
Multiple Exciton Generation in Si and Ge Nanoparticles with high pressure core structures — •Stefan Wippermann[1], Marton Vörös[2], Dario Rocca[3], Adam Gali[4], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Universite de Lorraine, Nancy — [4]Budapest University of Technology and Economics

Talk O 70.3 Thu 11:15 TRE Ma
Advanced time-evolution method for optical absorption spectra calculations — •Tobias Sander and Georg Kresse — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

Talk O 70.4 Thu 11:30 TRE Ma
New starting point for the calculation of optical properties — •Igor Reshetnyak[1,2] and Lucia Reining[1,2] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

Talk O 70.5 Thu 11:45 TRE Ma
Electron-Energy Loss and Inelastic X-ray Scattering of CuO from First Principles — •Claudia Rödl, Francesco Sottile, Matteo Gatti, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau cedex, France and European Theoretical Spectroscopy Facility (ETSF)

Talk O 70.6 Thu 12:00 TRE Ma

Optical Spectra from Molecules to Solids: Insight from Many-Body Perturbation Theory — •Caterina Cocchi and Claudia Draxl — Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

Talk O 70.7 Thu 12:15 TRE Ma
Relativistic Solar Cells — •Paolo Umari[1], Edoardo Mosconi[2], and Filippo De Angelis[2] — [1]Dipartimento di Fisica e Astronomia, Università di Padova, via Marzolo 8, I-35131 Padova, Italy — [2]Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM, Via Elce di Sotto 8, I-06123, Perugia, Italy

Talk O 70.8 Thu 12:30 TRE Ma
Solar nanocomposites with complementary charge extraction pathways for electrons and holes: Si embedded in ZnS — •Stefan Wippermann[1], Marton Vörös[2], Adam Gali[3], Francois Gygi[2], Gergely Zimanyi[2], and Giulia Galli[2] — [1]Max-Planck-Institute for Iron Research, Düsseldorf — [2]University of California, Davis — [3]Budapest University of Technology and Economics

Talk O 70.9 Thu 12:45 TRE Ma
Ultraviolet photo-emission spectroscopies from Koopmans-compliant functionals — •Ngoc Linh Nguyen[1], Giovanni Borghi[1], Andrea Ferretti[2], Ismaila Dabo[3], and Nicola Marzari[1] — [1]Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne, Station 12, 1015 Lausanne, Switzerland. — [2]Centro S3, CNR-Istituto Nanoscienze, I-41125 Modena, Italy — [3]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, USA.

Talk O 70.10 Thu 13:00 TRE Ma
Self-consistent dynamical embedding in real space — •Wael Chibani[1], Xinguo Ren[1,2], Patrick Rinke[1], and Matthias Scheffler[1] — [1]*Fritz Haber Institute of the Max Planck Society, Berlin, Germany* — [2]*Key Laboratory of Quantum Information, USTC, Hefei, China*