| Tuesday Oct. 11<br>Room: Napa A | | |
|---|---|---|
| 7:50-8:00AM | Opening Cerenomy | |
| **Session: DFT I Chair: Jianmin Tao** | | |
| 8:00-8:25AM | A01: A Fresh Look at the Band Gap Problem in Density Functional Theory | **John P. Perdew**<br>Temple University, USA |
| 8:25-8:50AM | A02: Free-energy DFT with Cost-effective Computational Scaling | **Sam Trickey**<br>University of Florida, USA |
| 8:50-9:15AM | A03: Ground-State Energy as a Simple Sum of Density Functional Orbital Energies | **Mel Levy**<br>Tulane University, USA |
| 9:15-9:40AM | A04: Power series approximation of the correlation kernel leading to Kohn-Sham methods combining accuracy, computational efficiency, and general applicability | **Andreas Görling**<br>University of Erlangen-Nuremberg, Germany |
| 9:40-10:05AM | A05: Approximating the exchange-correlation hole in the strong-interaction limit | **Matthias Ernzerhof**<br>University of Montreal, Canada |
| 10:05-10:20AM | Session Break | |
| **Session: General I Chair: Andy Teale** | | |
| 10:20 -10:45AM | A06: Relevance of Interface Region in Supported Nanocluster Catalysts | **Masahiro Ehara**<br>Institute for Molecular Science, Japan |
| 10:45-11:10AM | A07: Global and local curvature in density functional theory | **Heather Kulik**<br>Department of Chemical Engineering, MIT, USA |
| 11:10-11:35AM | A08: Proximity Effects on Topological Surface States of Bi2Se3 from First Principles | **Kyungwha Park**<br>Virginia Tech, USA |
| 11:35-12:00PM | A09: Molecular Conductivity and Conceptual Density Functional Theory | **Paul Geerlings**<br>Vrije Universiteit Brussel, Belgium |
| 12:00-12:25 PM | A10: Practical implementation of ensemble density functional theory: Basic aspect and applications | **Michael Filatov**<br>UNIST, Korea |
| 12:30-13:30 PM | Lunch Break | |

| Tuesday Oct. 11<br>Room: Napa A | | |
|---|---|---|
| **Session: General II Chair: Masahiro Ehara** | | |
| 13:30-13:55PM | A11: Current-density-functional theory, progress and challenges | **Andy Teale**<br>University of Nottingham, UK |
| 13:55 -14:20PM | A12: Coming to terms with computing the entropy of liquids from first principles | **Edmund R. Meyer**<br>Los Alamos National Laboratory, USA |
| 14:20 -14:45PM | A13: Density functional theory of electrons and nuclei without the Born-Oppenheimer approximation | **Ryan Requist**<br>Max Planck Institute of Microstructure Physics, Germany |
| 14:45 -15:10PM | A14: Design of New Disulfide-Based Organic Compounds for the Improvement of Self-Healing Materials[1] | **Jon M. Matxain**<br>UPV/EHU & DIPC, Spain |
| 15:10 -15:35PM | A15: Theoretical Challenges: From the 3d Transition Metals to the Heavy Elements | **Angela Wilson**<br>Michgan State University, USA |
| 15:35 -15:50PM | Session Break | |
| **Session: DFT II Chair: Andreas Görling** | | |
| 15:50 -16:15PM | A16: TBD | **Kieron Burke**<br>University of California-Ivine, USA |
| 16:15-16:40PM | A17: Recent progress on local hybrid functionals | **Martin Kaupp**<br>Technische Universität Berlin, Germany |
| 16:40-17:05PM | A18: Degeneracy, Convexity, and the Failures and Density Functional Theory | **Paul Ayers**<br>McMaster University, Canada |
| 17:05-17:30PM | A19: Spectacular success of DFT in predicting exotic topological phases of quantum matter | **Arun Bansil**<br>Northeastern University, USA |
| 17:30-17:55PM | A20: Reduction of Electronic Wave Functions to Exchange-Correlation Potentials | **Viktor Staroverov**<br>University of Western Ontario, Canada |

| Tuesday Oct. 11<br>Room: Huntington | | |
|---|---|---|
| **Session: Novel electron correlation methods for complex systems I Chair: Daniel Kats** | | |
| 13:30-13:55PM | H01: Quantum chemical treatment of crystalline fragments embedded in the periodic mean field | **Denis Usvyat**<br>University of Regensburg, Germany |
| 13:55 -14:20PM | H02: Distributed Gaussian Orbitals for Molecular Calculations | **Stefano Evangelisti**<br>Paul Sabatier University, France |
| 14:20 -14:45PM | H03: Amplitude Determinant Coupled Cluster Theory | **Eric Neuscamman**<br>University of California Berkeley, USA |
| 14:45 -15:10PM | H04: New Approaches for Strongly Correlated Electrons | **Mark Hoffmann**<br>University of North Dakota, USA |
| 15:10 -15:35PM | H05: Electron correlation effects in molecular crystals | **Carsten Müller**<br>Free University of Berlin, Germany |
| 15:35 -15:50PM | Session Break | |
| **Session: Oxide Electronics Chair: Ismaila Dabo** | | |
| 15:50 -16:15PM | H06: Theoretical spectroscopy of materials for oxide optoelectronics | **André Schleife**<br>University of Illinois, Urbana-Champaign, USA |
| 16:15-16:40PM | H07: Identification of vacancy defect complexes in transparent semiconducting oxides ZnO, In2O3 and SnO2 | **Ilja Makkonen**<br>Aalto University, Finland |
| 16:40-17:05PM | H08: Defect physics in oxides for electronics | **Anderson Janotti**<br>University of Delaware, USA |
| 17:05-17:30PM | H09: Resistivity switching in chalcogenide based interfacial phase change materials | **Nicki Frank Hinsche**<br>Technical University of Denmark, Denmark |
| 17:30-17:55PM | H10: Transition metal oxides in resistive switching | **Olle Heinonen**<br>Argonne National Laboratory, USA |

| Wednesday Oct. 12<br>Room: Napa A | | |
|---|---|---|
| **Session: DFT III Chair: Kieron Burke** | | |
| 8:25-8:50AM | A21: Löwdin Orthonormalized Fermi Orbitals for Self-Interaction-Corrected Density-Functional Approximations with Unitary Invariance | **Mark Pederson**<br>Johns Hopkins University, USA |
| 8:50-9:15AM | A22: Coulomb Descriptors - Euler Equation for Spherically Symmetric Systems | **Ágnes Nagy**<br>University of Debrecen, Hungary |
| 9:15-9:40AM | A23: Intrinsic Self-consistent Nature of the Schrödinger Equation for Electrons in Electromagnetic Fields | **Viraht Sahni**<br>CUNY Brooklyn College, USA |
| 9:40-10:05AM | A24: Semilocal density functional theory with correct surface asymptotics | **Lucian Constantin**<br>Italian Institute of Technology, Italy |
| 10:05-10:20AM | Session Break | |
| **Session: DFT IV Chair: Mark Pederson** | | |
| 10:20 -10:45AM | A25: Understanding the laser-induced spin dynamics in magnetic solids with non-collinear real-time TDDFT simulations | **Eberhard K. U. Gross**<br>Max Plank Institues, Germany |
| 10:45-11:10AM | A26: Currents through molecules from real time DFT: boundary conditions and exchange-correlation challenges | **Stephan Kuemmel**<br>Universität Bayreuth, Germany |
| 11:10-11:35AM | A27: Excitons in solids: TDDFT versus many-body perturbation theory | **Carsten Ullrich**<br>University of Missouri-Columbia, USA |
| 11:35-12:00PM | A28: Steady-State Density Functional Theory for Finite Bias Conductances | **Stefan Kurth**<br>Universidad del Pais Vasco UPV/EHU, Spain |
| 12:00-12:25PM | A29: Studying Aqueous Chemical Reactions from First Principles | **Evert Jan Meijer**<br>Universiteit van Amsterdam, Netherlands |
| 12:30-13:30PM | Lunch Break | |

| Wednesday Oct. 12<br>Room: Napa A | | |
|---|---|---|
| **Session: DFT V Chair: Stephan Kuemmel** | | |
| 13:30-13:55PM | A30: Time-dependent thermoelectric transport at the nanoscale | **Giovanni Vignale**<br>University of Missouri-Columbia, USA |
| 13:55 -14:20PM | A31: Development and Application of "Low-Cost" Dispersion Corrected Density Functional Methods | **Stefan Grimme**<br>University of Bonn, Germany |
| 14:20 -14:45PM | A32: TBD | **Adrienn Ruzsinszky**<br>Temple University, USA |
| 14:45 -15:10PM | A33: Making Density Functional Theory Work for All Materials | **Ann E. Mattsson**<br>Sandia National Laboratory, USA |
| 15:10-15:50PM | **Poster & Session Break** | |
| **Session: DFT VI Chair: Carsten Ullrich** | | |
| 15:50 -16:15PM | A34: Accurate Semilocal Density Functional and van der Waals Interaction | **Jianmin Tao**<br>Temple University, USA |
| 16:15-16:40PM | A35: TDDFT for Photochemistry | **John M. Herbert**<br>The Ohio State University, USA |
| 16:40-17:05PM | A36: First Principles Stochastic Approaches to Nanotechnology | **Roi Baer**<br>The Hebrew University of Jerusalem, Israel |
| 17:30-17:55PM | A37: Producing accurate equations of state based on density functional theory evaluated using the Dirac equation. | **John M. Wills**<br>Los Alamos National Laboratory, USA |

| Wednesday Oct. 12<br>Room: Napa B | | |
|---|---|---|
| **Session: Quantum Structure Chair: Anouar Benali** | | |
| 8:25-8:50AM | B01: Hemispheroidal microscopic model for investigation of nanoclusters deposited on a surface | **Dorin N Poenaru**<br>Horia Hulubei National Institute for Physics and Nuclear Engineering, Romania |
| 8:50-9:15AM | B02: Magnetic States of an Isotropic Magnet with the “Large” Ion Spin S = 3/2 ,1 | **Elena Orlenko**<br>Peter the Great St.Petersburg Polytechnic University, Russia |
| 9:15-9:40AM | B03: Recent Developments in DDEC Atomic Population Analysis | **Thomas A. Manz**<br>New Mexico State University, USA |
| 9:40-10:05AM | B04: Physical model for indium-rich InGaN/GaN quantum dot laser diodes | **Guan-Lin Su**<br>University of Illinois at Urbana-Champaign, USA |
| 10:05-10:20AM | Session Break | |
| 10:20 -10:45AM | B05: Pt(3D,1S) – O2 Interaction by ab initio Calculations | **Juan Horacio Pacheco-Sánchez**<br>Instituto Tecnológico de Toluca, México |
| 10:45-11:10AM | B06: First monohydrates of HCl•HNO3•H2SO4 aggregates: geometries, spectra and atmospheric behavior | **Marian Verdes**<br>Universidad Autónoma de Madrid, Spain |
| **Session: Quantum Monte Carlo I Chair: Elena Orlenko** | | |
| 11:10-11:35AM | B07: Monte Carlo Configuration Interaction: Multireference measures, positronic molecules and open-shell systems. | **Jeremy Coe**<br>Heriot-Watt University, UK |
| 11:35-12:00PM | B08: From multi-reference Trial Wavefunction to Fragmented Molecular Orbitals for Quantum Monte Carlo: Accuracy versus system-size | **Anouar Benali**<br>Argonne National Laboratory, USA |
| 12:00-12:25PM | B09: Systematic study of transition metal oxides with diffusion Monte Carlo | **Jaron T. Krogel**<br>Oak Ridge National Laboratory, USA |
| 12:30-13:30PM | Lunch Break | |

| Wednesday Oct. 12<br>Room: Napa B | | |
|---|---|---|
| **Session: Molecular Dynamics and its applications Chair: Ioan Baldea** | | |
| 13:30-13:55PM | B10: Structural order in nanofluidic materials | **Itsuo Hanasaki**<br>Tokyo University of Agriculture and Technology, Japan |
| 13:55 -14:20PM | B11: Simulation of the interaction of hydrogen with metal nanoparticles supported on graphene substrates | **Julio A. Alonso**<br>University of Valladolid, Spain |
| 14:20 -14:45PM | B12: Quantum dynamics study on electron attachment to molecules and clusters | **Toshiyuki Takayanagi**<br>Saitama University, Japan |
| 14:45 -15:10PM | B13: Solvation Motor: A New and Simple Model of Motor Proteins | **Ken Tokunaga**<br>Division of Liberal Arts, Kogakuin University, Japan |
| 15:10-15:50PM | **Poster & Session Break** | |
| 15:50 -16:15PM | B14: Graphene trumpets, foams, pillared networks, carbon materials growth, and all that from first-principles | **Simone Taioli**<br>ECT*, Italy&<br>Charles University in Prague, Czech Republic |
| 16:15-16:40PM | B15: Electron Nuclear Dynamics Simulations of Water Radiolysis and DNA Damage in Proton Cancer Therapy | **Jorge A. Morales**<br>Texas Tech University, USA |
| 16:40-17:05PM | B16: First-Principles Prediction of the Electrochemical Stability of Bimetallic Catalysts for Use as Fuel Cell Electrodes | **Ismaila Dabo**<br>The Pennsylvania State University, USA |
| **Session: Molecular Electronics Chair: Julio A. Alonso** | | |
| 17:05-17:30PM | B17: Exciton Dynamics in DNTT Thin Films | **Takatoshi Fujita**<br>Institute for Molecular Science, Japan |
| 17:30-17:55PM | B18: Universality Out of Equilibrium. A Law of Corresponding States for Charge Transport Via Tunneling in Molecular Junctions | **Ioan Baldea**<br>Universitaet Heidelberg, Germany |

| Wednesday Oct. 12<br>Room: Napa C | | |
|---|---|---|
| **Session: Novel electron correlation methods for complex systems II Chair: Denis Usvyat** | | |
| 8:00-8:25AM | C01: Stochastic-CASSCF and Multi-Configuration Pair-Density Functional Theory: A New Era for Strongly Correlated Molecular Systems | **Giovanni Li Manni**<br>Max Planck Insitute for Solid State Research, Stuttgart, Germany |
| 8:25-8:50AM | C02: The Tortoise and the Hare: Canonical and Local MP2 Implementations for Periodic Systems | **Lorenzo Maschio**<br>University of Turin, Italy |
| 8:50-9:15AM | C03: Accurate coupled cluster calculations for the high multiplicity states | **Monika Musiał**<br>University of Silesia, Poland |
| 9:15-9:40AM | C04: Recent Progress in the Electron-Attached, Ionized, and Active-Space Equation-of-Motion Coupled-Cluster Methodologies | **Piotr Piecuch**<br>Michigan State University, USA |
| 9:40-10:05AM | C05: Newest developments of the method of increments for strongly correlated systems | **Edoardo Fertitta**<br>Free University of Berlin, Germany |
| 10:05-10:20AM | Session Break | |
| **Session: General III Chair: Thorsten Klüner** | | |
| 10:20 -10:45AM | C06: In search of unconventional ultrathin metastable O/Cu surface oxides | **Aloysius Soon**<br>Yonsei University, Korea |
| 10:45-11:10AM | C07: Transport properties of correlated metals: A dynamical mean field theory perspective | **Xiaoyu Deng**<br>Rutgers University, USA |
| 11:10-11:35AM | C08: Assigning the cerium oxidation state in complexes by multireference wavefunction analysis | **Oliver Moossen**<br>Universität zu Köln, Germany |
| 11:35-12:00PM | C09: On the origin of cooperativity in hydrogen bonding | **Joe Ireta**<br>Universidad Autónoma Metropolitana-Iztapalapa, Mexico |
| 12:00-12:25PM | C10: The Praxis of Theory & Experiment in the Study of Non-Covalent Interactions in Organometallics | **Jean-Pierre Djukic**<br>University of Strasbourg, France |
| 12:30-13:30PM | Lunch Break | |

| Wednesday Oct. 12<br>Room: Napa C | | |
|---|---|---|
| **Session: General IV Chair: Dorothée Berthomieu** | | |
| 13:30-13:55PM | C11: Hybrid quantum-classical dynamics simulation of interface bonding between epoxy resin and oxidized aluminum | **Shuji Ogata**<br>Nagoya Institute of Technology, Japan |
| 13:55 -14:20PM | C12: A first principles approach to the photoreactivity of oxide surfaces | **Thorsten Klüner**<br>University of Oldenburg, Germany |
| 14:20 -14:45PM | C13: Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods | **Noa Marom**<br>Carnegie Mellon University, USA |
| 14:45 -15:10PM | C14: DFT approaches for graphene based materials for energy applications | **Marika Savarese**<br>Istituto Italiano di Tecnologia (IIT), Italy |
| 15:10-15:50PM | **Poster & Session Break** | |
| **Session: General V Chair: Oliver Moossen** | | |
| 15:50 -16:15PM | C15: Structures and spectroscopic properties of coordination polymers using DFT | **Dorothée Berthomieu**<br>Institut Charles Gerhardt Montpellier, France |
| 16:15-16:40PM | C16: Inter- and intramolecular interactions from Kohn-Sham random-phase approximation correlation methods including exchange contributions | **Andreas Hesselmann**<br>Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany |
| 16:40-17:05PM | C17: Electron-phonon interactions and electrical and thermal transport in graphene | **Cheol-Hwan Park**<br>Seoul National University, Korea |
| 17:05-17:30PM | C18: Orbital-free DFT approaches to equation of state and transport properties for warm dense matter | **Travis Sjostrom**<br>Los Alamos National Laboratory, USA |
| 17:30-17:55PM | C19: Design and density functional theory explorations on the luminescent mechanism of AuCu nanoclusters | **Haizhu Yu**<br>Anhui University, China |

| Thursday Oct. 13<br>Room: Napa A | | |
|---|---|---|
| **Session: Recent advances in theoretical spectroscopy I  Chair: Xinguo Ren** | | |
| 8:25-8:50AM | A38: Modeling Absorption and Emission Spectra of Large Organic Dyes with Double-Hybrid Density-Functionals | **Eric Brémond**<br>Istituto Italiano di Tecnologia (IIT), Italy |
| 8:50-9:15AM | A39: A Combined Experimental and Theoretical Studies on Circular Dichroisms of Propeller Chirality of Hexaarylbenzenes and Related Molecules | **Tadashi Mori**<br>Osaka Univeristy, Japan |
| 9:15-9:40AM | A40: Local representation of the response function: Theory and applications | **Deyu Lu**<br>Brookhaven National Laboratory, USA |
| 9:40-10:05AM | A41: To GW and beyond -- from weak to strong correlation | **Patrick Rinke**<br>Aalto University, Finland |
| 10:05-10:20AM | Session Break | |
| **Session: Novel electron correlation methods for complex system III  Chair: Daniel Kats** | | |
| 10:20 -10:45AM | A42: Electron correlation by polarization of interacting densities | **Jerry L. Whitten**<br>North Carolina State University, USA |
| 10:45-11:10AM | A43: Projection-based wavefunction-in-DFT embedding | **Fred Manby**<br>University of Bristol, UK |
| 11:10-11:35AM | A44: Large-scale v2RDM-driven CASSCF methods | **A. Eugene DePrince III**<br>Florida State University, USA |
| 11:35-12:00PM | A45: Static and dynamical electron correlation calculations of large systems based on the divide-and-conquer method | **Masato Kobayashi**<br>Hokkaido University, Japan |
| 12:00-12:25PM | A46: TBD | **Edward Valeev**<br>Virginia Tech, USA |
| 12:30-13:30PM | Lunch Break | |

| Thursday Oct. 13<br>Room: Napa A | | |
|---|---|---|
| **Session: DFT VII Chair: Ann E. Mattsson** | | |
| 13:30-13:55PM | A47: Ab initio thermodynamic approach to identify and design materials for CO2 Capture Technologies | **Yuhua Duan**<br>US DOE-National Energy Technology Laboratory, USA |
| 13:55 -14:20PM | A48: Second-Order Perturbation Theory for Fractional Occupation Systems: Applications to IP and EA Calculations | **Xin Xu**<br>Fudan Univeristy, China |
| 14:20 -14:45PM | A49: TBD | **Roberto Car**<br>Princeton University, USA |
| 14:45 -15:10PM | A50: Electrochemistry at electrode/electrolyte interfaces from first principles | **Axel Gross**<br>Ulm University, Germany |
| 15:10 -15:35PM | A51: Accurate Excitation Energy, Reaction Barrier Height, and Enthalpy of Reaction from Semilocal Density Functionals | **Guocai Tian**<br>Kunming University of Science and Technology, China |
| 15:35-15:50PM | **Session Break** | |
| **Session: Recent advances in theoretical spectroscopy II Chair: Patrick Rinke** | | |
| 15:50 -16:15PM | A52: Adaptively compressed exchange operator | **Lin Lin**<br>University of California, Berkeley, USA |
| 16:15-16:40PM | A53: Accurate X-Ray Absorption Predictions for Transition Metal Oxides: An Advanced Self-Consistent Approach Inspired by Many-Body Perturbation Theory | **David Prendergast**<br>Theory of Nanostructured Materials Facility, Molecular Foundry, USA |
| 16:40-17:05PM | A54: Spectroscopic properties of materials from many-body perturbation theory | **Sahar Sharifzadeh**<br>Boston University, USA |
| 17:05-17:30PM | A55: First-principles calculations and model analysis of plasmon excitations in graphene | **Xinguo Ren**<br>University of Science and Technology of China, China |

| Thursday Oct. 13<br>Room: Napa B | | |
|---|---|---|
| **Session: Moller–Plesset perturbation theory and Coupled-Cluster Theory Chair: Tzonka Mineva** | | |
| 8:00-8: 25AM | B19: Correlated wave functions from spin-extended Hartree-Fock | **Takashi Tsuchimochi**<br>Kobe University, Japan |
| 8:25-8:50AM | B20: Novel Coupled-Cluster approaches for heavy element chemistry | **Katharina Boguslawski**<br>Nicolaus Copernicus University, Poland |
| 8:50-9:15AM | B21: Ab Initio and Semi-Empirical Quantum Chemistry Studies of Partial-Oxidation Processes in Spin Traps | **Scott Kirkby**<br>East Tennessee State University, USA |
| 9:15-9:40AM | B22: TBD | **Thomas Bondo Pedersen**<br>University of Oslo, Norway |
| 9:40-10:05AM | B23: Many-Body Density Matrix Theory | **Christopher J. Tymczak**<br>Texas Southern University, USA |
| 10:05-10:20AM | Session Break | |
| **Session: NMR Calculation Chair: Scott Kirkby** | | |
| 10:20 -10:45AM | B24: Computation of NMR quantities by means of Stochastic Liouville Equation | **Danuta Kruk**<br>University of Warmia and Mazury in Olsztyn, Poland |
| 10:45-11:10AM | B25: Dynamic NMR parameters to study organic-inorganic interfaces in templated materials | **Tzonka Mineva**<br>Institut Charles Gerhardt, Montpellier, France |
| 11:10-11:35AM | B26: Using ab initio fragmentation methods for the prediction of NMR spectra | **Rika Kobayashi**<br>ANU Supercomputer Facility, Australia |
| 11:35-13:55PM | Lunch Break | |

| Thursday Oct. 13<br>Room: Napa B | | |
|---|---|---|
| **Session: Quantum Monte Carlo II Chair: Thomas Bondo Pedersen** | | |
| 13:55-14:20PM | B27: Quantum Monte Carlo simulations of molecular interactions using high performance computing | **Kenta Hongo**<br>Japan Advanced Institute of Science and Technology, Japan |
| 14:20-14:45PM | B28: Non-Orthogonal Slater Determinant Expansions in Quantum Monte Carlo | **Miguel Morales-Silva**<br>Lawrence Livermore National Laboratory, USA |
| 14:45-15:10PM | B29: Hybridization of Quantum Monte Carlo and Effective Fragment Molecular Orbital methods, and the nodal variational principle | **Federico Zahariev**<br>Iowa State University, USA |
| 15:10-15:35PM | B30: Selected CI wavefunctions for Diffusion Monte Carlo | **Michel Caffarel**<br>CNRS-Lab. de Chimie et Physique Quantiques, France |
| 15: 35-15:50PM | **Session Break** | |
| **Session: Novel electron correlation methods for complex systems IV Chair: Denis Usvyat** | | |
| 15:50 -16:15PM | B31: ADDTION BY SUBTRACTION IN COUPLED-CLUSTER THEORY | **Rodney Bartlett**<br>University of Florida, USA |
| 16:15-16:40PM | B32: TBD | **Garnet Chan**<br>Princeton University, USA |
| 16:40-17:05PM | B33: On the perturbative computation of ionization energies | **Peter Knowles**<br>Cardiff University, UK |
| 17:05-17:30PM | B34: Electron Correlation: Citius, Altius, Fortius | **Daniel Kats**<br>Universität Stuttgart, Germany |

| Thursday Oct. 13<br>Room: Napa C | | |
|---|---|---|
| **Session: General VI Chair: Noa Marom** | | |
| 8:00-8:25AM | C20: Towards reliable modeling of electronic structures and spectroscopic parameters of uranium oxides | **Paweł Tecmer**<br>Nicolaus Copernicus University, Poland |
| 8:25-8:50AM | C21: Non-empirically tuned long-range corrected hybrid functionals for organic electronic materials | **Thomas Körzdörfer**<br>University of Potsdam, Germany |
| 8:50-9:15AM | C22: First-Principles Study of The Electronic Structure in Molecular Conductors with Hybrid Functional | **Takao Tsumuraya**<br>National Institute for Materials Science, Japan |
| 9:15-9:40AM | C23: DFT simulations on million-atom systems using a linear-scaling DFT code CONQUEST | **Tsuyoshi Miyazaki**<br>Institute for Materials Science, Japan |
| 9:40-10:05AM | C24: Density-functional theory and experiment: a match made in heaven or in hell? | **Kurt Lejaeghere**<br>Ghent University, Belgium |
| 10:05-10:20AM | Session Break | |
| **Session: General VII Chair: Thomas Körzdörfer** | | |
| 10:20 -10:45AM | C25: Computational screening of hydrogen storage materials with density functional theory | **Adem Tekin**<br>Istanbul Technical University, Turkey |
| 10:45-11:10AM | C26: Dark Photo-Switching of a Dihydroazulene Derivative in the Coulomb Blockade Regime | **Stine T. Olsen**<br>University of Copenhagen, Denmark |
| 11:10-11:35AM | C27: Electron-phonon coupling beyond semilocal DFT | **Bartomeu Monserrat**<br>Rutgers University and University of Cambridge, UK |
| 11:35-11:50AM | C28: Understanding the advantage of hexagonal WO3 as an efficient photoanode for solar water splitting: A first-principles perspective | **Yonghyuk Lee**<br>Yonsei University, Korea |
| 11:50-13:30PM | Lunch Break | |

| Thursday Oct. 13<br>Room: Napa C | | |
|---|---|---|
| **Session: General VIII Chair: Kurt V. Mikkelsen** | | |
| 13:30-13:55PM | C29: Electron Density Analysis of Heavy Elements | **Julien Pilmé**<br>Pierre-and-Marie-Curie University, France |
| 13:55-14:20PM | C30: Electron-state Tuning of MoS2 Thin Film by Electrostatic and Chemical Doping | **Nguyen Thanh Cuong**<br>NIMS, Japan |
| 14:20-14:45PM | C31: Photo-excited Dynamics at Nanoscale Interfaces | **Run Long**<br>Beijing Normal University, China |
| 14:45-15:10PM | C32: Using Computational Materials Chemistry to Tackle Industrial Problems: Successes and Challenges | **Glenn Jones**<br>Johnson Matthey Technology Centre, South Africa |
| 15:10-15:35PM | C33: Nonadiabatic dynamics of condensed phase proton-coupled electron transfer reactions | **Gabriel Hanna**<br>University of Alberta, Canada |
| 15: 35-15:50PM | **Session Break** | |
| **Session: General Ⅸ Chair: Gabriel Hanna** | | |
| 15:50 -16:15PM | C34: A MODEL FOR SOLAR HEATING | **Kurt V. Mikkelsen**<br>University of Copenhagen, Denmark |
| 16:15-16:40PM | C35: Transition States of Spin-State Crossing Reactions | **Jun-ya Hasegawa**<br>Hokkaido University, Japan |
| 16:40-17:05PM | C36: Accurate potentials and dynamics: current status | **António Varandas**<br>Universidade de Coimbra, Portugal |
| 17:05-17:30PM | C37: Photochromic Diarylethenes as Photoactivatable Drugs | **José Pedro Cerón-Carrasco**<br>UCAM Campus de los Jerónimos, Spain |
| 17:30-17:55PM | C38: Exchange-like Kernel Corrections within RPA Renormalization | **Jefferson Bates**<br>Temple University, USA |
| 17:55-18:10PM | C39: Acute mechano-electronic responses in twisted phosphorene nanoribbons | **Woosun Jang**<br>Yonsei University, Korea |

| **Wednesday Oct. 12**<br>**Poster session** (15:10-15:50PM) | | |
|---|---|---|
| P01 | Calibration of Exchange Energy Density in Local Hybrid Functionals: Recent Developments | **Alexey Arbuznikov**<br>Department of Chemistry, TU Berlin, Germany |
| P02 | Luminescent bi-nuclear Cu(I) complexes as potential TADF emitters: A theoretical study | **David Ambrosek**<br>CYNORA GmbH, Germany |
| P03 | Computational serach for sulphide perovskites for solar energy conversion application | **Korina Kuhar**<br>Technical University of Denmark, Denmark |
| P04 | Amplitude Determinant Coupled Cluster Theory | **Luning Zhao**<br>University of California, Berkeley, USA |
| P05 | Studying some fundamental concepts of DFT with an accurate wavefunction for two-electron systems | **Rabeet Singh Chauhan**<br>Indian Institute of Technology Kanpur, India |
| P06 | One-atom thick h-CrN: Electronic Properties and Synthesis Recommendations | **Artem Kuklin**<br>Kyungpook National University, Korea |
| P07 | Developing an Atomic Population Analysis Suitable for Use as a Default Method in Quantum Chemistry Programs | **Nidia Gabaldon Limas**<br>New Mexico State University, USA |
| P08 | DFT applied to Transition Metal Elements and Binaries: Development of The V-DM/16 Test Set | **Elizabeth Decolvenaere**<br>University of California: Santa Barbara , USA |
| P09 | First Principles Crystal Structure Prediction for Dual Cation Ammine Metal Borohydrides | **Samet Demir**<br>Istanbul Technical University, Turkey |
| P10 | DFT Calculations of Thermodynamic Properties of II-VI and IV-VI Crystals | **Bohdanna Volochanska**<br>Vasyl Stefanyk Precarpathian National University, Ukraine |
| P11 | Number Counting Jastrow Factors in Real Space | **Brett Van Der Goetz**<br>University of California, Berkeley, USA |