

Session Index

Session A1: Recent Advances in Density Functional Theory I

Sponsoring Units: DCP DCOMP

Chair: Weitao Yang, Duke University

Room: 103/105

Monday, March 3, 2014
8:00AM - 8:36AM

[A1.00001: Strong Correlation in Density-Functional Theory](#)

Invited Speaker: Axel Becke

Monday, March 3, 2014
8:36AM - 8:48AM

[A1.00002: Strong correlation in Kohn-Sham DFT](#)

Francesc Malet Giralt , Andr e Mirtschink , Jonas Cremon , Christian Mendl , Klaas Giesbertz , Stephanie Reimann , Paola Gori-Giorgi

Monday, March 3, 2014
8:48AM - 9:00AM

[A1.00003: Local Correction to Reduce Delocalization Errors in Approximate Density Functionals](#)

Chen Li , Xiao Zheng , Weitao Yang

Monday, March 3, 2014
9:00AM - 9:12AM

[A1.00004: Density-driven delocalization error for a model solvated electron system](#)

Stephen Dale , Alberto Otero-de-la-Roza , Erin Johnson

Monday, March 3, 2014
9:12AM - 9:48AM

[A1.00005: Gedanken Densities and Lower Bounds in Density Functional Theory](#)

Invited Speaker: John P. Perdew

Monday, March 3, 2014
9:48AM - 10:00AM

[A1.00006: First beyond-LSDA density functional satisfying a tight lower bound for exchange](#)

Jianwei Sun , John Perdew , Adrienn Ruzsinszky

Monday, March 3, 2014
10:00AM - 10:12AM

[A1.00007: Band gaps with approximate density functionals: the derivative discontinuity revealed from ensemble considerations](#)

Eli Kraisler , Leeor Kronik

Monday, March 3, 2014
10:12AM - 10:24AM

[A1.00008: Gap renormalization of molecular crystals from density-functional theory](#)

Sivan Refaely-Abramson , Sahar Sharifzadeh , Manish Jain , Roi Baer , Jeffrey B. Neaton , Leeor Kronik

Monday, March 3, 2014
10:24AM - 10:36AM

[A1.00009: Local Density Approximation Exchange-correlation Free-energy Functional](#)

Valentin Karasiev , Travis Sjostrom , James Dufty , S.B. Trickey

Monday, March 3, 2014
10:36AM - 10:48AM

[A1.00010: Constrained Parameterization of Reduced Density Approximation of Kinetic Energy Functionals](#)

Debajit Chakraborty , Samuel Trickey , Valentin Karasiev

Monday, March 3, 2014
10:48AM - 11:00AM

[A1.00011: Modeling Electron Correlation Using Geminal Hybrid Methods](#)

Brett Cagg , Vitaly Rassolov

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Session B1: Recent Advances in Density Functional Theory II

Sponsoring Units: DCP DCOMP

Chair: Viktor Staroverov, University of Western Ontario (Canada)

Room: 103/105

Monday, March 3, 2014 11:15AM - 11:27AM	B1.00001: Correlation Energy of the Homogeneous Electron Gas from Adiabatic Connection Fluctuation-Dissipation Theory including Exact Exchange kernel Nicola Colonna , Stefano de Gironcoli
Monday, March 3, 2014 11:27AM - 11:39AM	B1.00002: Molecular dissociation within the adiabatic connection fluctuation dissipation framework Maria Hellgren , Nicola Colonna , Stefano de Gironcoli
Monday, March 3, 2014 11:39AM - 11:51AM	B1.00003: Coupled-Cluster and Linear-Response Time-Dependent Density-Functional Theory Perspectives on Particle-Particle Random-Phase Approximation Degao Peng , Helen van Aggelen , Stephan Steinmann , Yang Yang , Weitao Yang
Monday, March 3, 2014 11:51AM - 12:27PM	B1.00004: Exchange-correlation energies from pairing matrix fluctuations and the particle-particle Random Phase Approximation Invited Speaker: Helen van Aggelen
Monday, March 3, 2014 12:27PM - 12:39PM	B1.00005: Double, Rydberg and Charge Transfer Excitations from Pairing Matrix Fluctuation and Particle-Particle Random Phase Approximation Yang Yang , Helen van Aggelen , Weitao Yang
Monday, March 3, 2014 12:39PM - 12:51PM	B1.00006: Dynamical second-order Bethe-Salpeter equation kernel: a method for electronic excitation beyond the adiabatic approximation Du Zhang , Stephan Steinmann , Weitao Yang
Monday, March 3, 2014 12:51PM - 1:03PM	B1.00007: On the Edge of Koopmans' Theorem Paul Grabowski , Kieron Burke
Monday, March 3, 2014 1:03PM - 1:39PM	B1.00008: DFT calculations with the exact functional Invited Speaker: Kieron Burke
Monday, March 3, 2014 1:39PM - 1:51PM	B1.00009: Uniform semiclassical approximations for many-particle systems Raphael Ribeiro , Kieron Burke
Monday, March 3, 2014 1:51PM - 2:03PM	B1.00010: Benchmarking Density Functional Theory with Density Matrix Renormalization Group and Lessons For Higher Dimensions Thomas E. Baker , Lucas O. Wagner , E. Miles Stoudenmire , Steven R. White , Kieron Burke
Monday, March 3, 2014 2:03PM - 2:15PM	B1.00011: Ensemble density-functional theory for excited states: exact results versus approximations Zenghui Yang , Aurora Pribram-Jones , Kieron Burke , Richard Needs , Carsten Ullrich

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Session G1: Recent Advances in Density Functional Theory III

Sponsoring Units: DCP DCOMP

Chair: John P. Perdew, Temple University

Room: 103/105

Tuesday, March 4, 2014 11:15AM - 11:51AM	G1.00001: Insight into Structural Phase Transitions from Density Functional Theory Invited Speaker: Adrienn Ruzsinszky
Tuesday, March 4, 2014 11:51AM - 12:03PM	G1.00002: New ways of computing effective potentials for orbital-dependent functionals Viktor N. Staroverov
Tuesday, March 4, 2014 12:03PM - 12:15PM	G1.00003: Rationalization of Hubbard U in CeOx from first principles: Unveiling the role of local structure in screening Deyu Lu , Ping Liu
Tuesday, March 4, 2014 12:15PM - 12:27PM	G1.00004: Adiabatic Connection and Virial Theorem for Ensemble Density Functional Theory Aurora Pribram-Jones , Zeng-hui Yang , Carsten Ullrich , Richard Needs , Kieron Burke
Tuesday, March 4, 2014 12:27PM - 1:03PM	G1.00005: Hybrid Density Functionals Tuned towards Fulfillment of Fundamental DFT Conditions Invited Speaker: Matthias Scheffler
Tuesday, March 4, 2014 1:03PM - 1:15PM	G1.00006: Performance of optimally-tuned range-separated hybrid functionals in predicting molecular valence-electron spectra David A. Egger , Shira Weissman , Sivan Refaely-Abramson , Sahar Sharifzadeh , Matthias Dauth , Roi Baer , Stephan Kuemmel , Jeffrey B. Neaton , Egbert Zojer , Leor Kronik
Tuesday, March 4, 2014 1:15PM - 1:27PM	G1.00007: Electronic structure of CuPc from an optimally-tuned range-separated hybrid functional Shira Weissman , Sivan Refaely-Abramson , David A. Egger , Egbert Zojer , Leor Kronik
Tuesday, March 4, 2014 1:27PM - 1:39PM	G1.00008: Kinetic and Hole Contributions to the Exact TDDFT Correlation Potential Kai Luo , Johanna Fuks , Ernesto Sandoval , Peter Elliott , Neepa Maitra
Tuesday, March 4, 2014 1:39PM - 1:51PM	G1.00009: First-Principles Studies of the Excited States and Optical Properties of Xanthene Derivative Chromophores Samia Hamed , Sahar Sharifzadeh , Jeffrey Neaton
Tuesday, March 4, 2014 1:51PM - 2:03PM	G1.00010: Exact Factorization of the Electron-Nuclear Wavefunction: Exact Electronic Potentials in Coupled Electron-Ion Dynamics Yasumitsu Suzuki , Ali Abedi , Neepa T. Maitra , Koichi Yamashita , E.K.U. Gross
Tuesday, March 4, 2014 2:03PM - 2:15PM	G1.00011: Exact factorization of the electron-nuclear wave function: Is the Berry phase an artefact of the Born-Oppenheimer approximation? Seung Kyu Min , Ali Abedi , E.K.U. Gross , Kwang S. Kim

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Session J1: Recent Advances in Density Functional Theory IV

Sponsoring Units: DCP DCOMP

Chair: Neepa Maitra, Hunter College

Room: 103/105

Tuesday, March 4, 2014 2:30PM - 3:06PM	J1.00001: Towards accurate density-functional treatment of non-covalent interactions in complex systems Invited Speaker: Erin Johnson
Tuesday, March 4, 2014 3:06PM - 3:18PM	J1.00002: Optimization of van der Waals Density Functionals using Data Projection onto Parameter Space (DPPS) Michelle Fritz , Marivi Fernandez-Serra , Mike Gillan , Jose M. Soler
Tuesday, March 4, 2014 3:18PM - 3:30PM	J1.00003: Electronic Properties of Surfaces and Interfaces with Self-Consistent van der Waals Density Functional Nicola Ferri , Robert A. DiStasio Jr. , Roberto Car , Alexandre Tkatchenko , Matthias Scheffler
Tuesday, March 4, 2014 3:30PM - 3:42PM	J1.00004: Van der Waals Interactions: Beyond Energies Alexandre Tkatchenko
Tuesday, March 4, 2014 3:42PM - 4:18PM	J1.00005: Recent Developments in Fragment-based Density Functional Theory Invited Speaker: Adam Wasserman
Tuesday, March 4, 2014 4:18PM - 4:30PM	J1.00006: Ab-initio Charge and Spin Dynamics in Solids using TDDFT Peter Elliott , K Krieger , S Sharma , J.K Dewhurst , E.K.U Gross
Tuesday, March 4, 2014 4:30PM - 4:42PM	J1.00007: Ensemble treatment of fragments within a molecule leads to improved description of dissociation Jonathan Nafziger , Adam Wasserman
Tuesday, March 4, 2014 4:42PM - 4:54PM	J1.00008: Practical methods in time-dependent density functional theory (TDDFT) at elevated temperatures Rudolph Magyar , Luke Shulenburger , Andrew Baczewski
Tuesday, March 4, 2014 4:54PM - 5:06PM	J1.00009: Recovering the Integer Discontinuity of Density Functional Approximations Martin Mosquera , Adam Wasserman
Tuesday, March 4, 2014 5:06PM - 5:18PM	J1.00010: Modeling long-range time-resolved charge-transfer within TDDFT: Insights from a 2-site lattice model Johanna Fuks , Neepa Maitra
Tuesday, March 4, 2014 5:18PM - 5:30PM	J1.00011: Time-Resolved Dynamics in Exact TDDFT: Studies of Two-Electron Systems Ernesto Sandoval , Johanna Fuks , Kai Luo , Neepa Maitra , Peter Elliott

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Session L1: Recent Advances in Density Functional Theory V

Sponsoring Units: DCP DCOMP

Chair: Aurora Pribram-Jones, University of California, Irvine

Room: 103/105

Wednesday, March 5, 2014 8:00AM - 8:36AM	L1.00001: Recent progress in density functional theory Invited Speaker: Donald Truhlar
Wednesday, March 5, 2014 8:36AM - 8:48AM	L1.00002: Density-Decomposed Orbital-Free Density Functional Theory for Covalent Systems and Application to Li-Si alloys Junchao Xia , Emily Carter
Wednesday, March 5, 2014 8:48AM - 9:00AM	L1.00003: Density-Functional Theory of Thermal Transport F.G. Eich , A. Principi , M. Di Ventra , G. Vignale
Wednesday, March 5, 2014 9:00AM - 9:12AM	L1.00004: Accurate and systematically improvable quantum embedding methods for complex systems Jason Goodpaster , Taylor Barnes , Frederick Manby , Thomas Miller
Wednesday, March 5, 2014 9:12AM - 9:48AM	L1.00005: Wavefunctions, Adiabatic Connections, and Universal Functionals for 1-Matrix Functional Theory Invited Speaker: Paul Ayers
Wednesday, March 5, 2014 9:48AM - 10:00AM	L1.00006: Semiclassical approach to the exchange energy from potential functional theory Attila Cangi , Peter Elliott , Stefano Pittalis , E.K.U. Gross , Kieron Burke
Wednesday, March 5, 2014 10:00AM - 10:12AM	L1.00007: Three- to two-dimensional crossover in time-dependent density-functional theory Shahrzad Karimi , Carsten Ullrich
Wednesday, March 5, 2014 10:12AM - 10:24AM	L1.00008: Stationary state Kohn-Sham Theory: Modern algorithms breathe new life into an old theory Deniz Gunceler , Ravishankar Sundararaman , T.A. Arias
Wednesday, March 5, 2014 10:24AM - 10:36AM	L1.00009: Increasing the efficiency and accuracy of time-resolved electronic spectra calculations with on-the-fly ab initio quantum dynamics methods Jiri Vanicek
Wednesday, March 5, 2014 10:36AM - 10:48AM	L1.00010: Exploring Nuclear Effects in the Dynamics of Nanomaterials with a Quantum Trajectory-Electronic Structure Approach Sophya Garashchuk

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Session M1: Recent Advances in Density Functional Theory VI

Sponsoring Units: DCP DCOMP

Chair: Jianwei Sun, Temple University

Room: 103/105

Wednesday, March 5, 2014 11:15AM - 11:51AM	M1.00001: The derivative discontinuity of the exchange-correlation functional Invited Speaker: Aron Cohen
Wednesday, March 5, 2014 11:51AM - 12:03PM	M1.00002: Hohenberg-Kohn Theorem Including Electron Spin in the Presence of a Magnetostatic Field Viraht Sahni , Xiao-Yin Pan
Wednesday, March 5, 2014 12:03PM - 12:15PM	M1.00003: Wigner High Electron Correlation Regime of Nonuniform Electron Density Systems: A Quantal Density Functional Theory (QDFT) Study Doug Achan , Lou Massa , Viraht Sahni
Wednesday, March 5, 2014 12:15PM - 12:27PM	M1.00004: Magnetic Orders of LaTiO₃ and YTiO₃ Under Epitaxial Strain: a First-Principles study Yakui Weng , Xin Huang , Yankun Tang , Shuai Dong
Wednesday, March 5, 2014 12:27PM - 12:39PM	M1.00005: Testing the Standard Approach for Density-Functional Transport Calculations Justin Smith , Zhenfei Liu , Kieron Burke
Wednesday, March 5, 2014 12:39PM - 12:51PM	M1.00006: Quantum oscillations in the kinetic energy density: Gradient corrections from the Airy gas Alexander Lindmaa , Ann E. Mattsson , Rickard Armiento
Wednesday, March 5, 2014 12:51PM - 1:03PM	M1.00007: Nuclear Quantum Effects in Liquid Water: A Highly Accurate <i>ab initio</i> Path-Integral Molecular Dynamics Study Robert A. DiStasio Jr. , Biswajit Santra , Hsin-Yu Ko , Roberto Car
Wednesday, March 5, 2014 1:03PM - 1:15PM	M1.00008: Gutzwiller density functional theory for solid hydrogen calculations Jun Liu , Yongxin Yao , Chen Liu , Wencai Lu , Cai-zhuang Wang , Kai-Ming Ho
Wednesday, March 5, 2014 1:15PM - 1:27PM	M1.00009: Understanding Machine-learned Density Functionals Li Li , John Snyder , Matthias Rupp , Klaus-Robert Müller , Kieron Burke
Wednesday, March 5, 2014 1:27PM - 1:39PM	M1.00010: Relation of exact Gaussian basis methods to the dephasing representation: Theory and application to time-resolved electronic spectra Miroslav Sulc , Henar Hernandez , Todd J. Martinez , Jiri Vanicek
Wednesday, March 5, 2014 1:39PM - 1:51PM	M1.00011: Exorcising Ghost Transmission from Electron Transport Calculations: Refighting Old Battles in New Contexts Matthew Reuter , Robert Harrison
Wednesday, March 5, 2014 1:51PM - 2:03PM	M1.00012: Green's functions in equilibrium and nonequilibrium from real-time bold-line Monte Carlo Guy Cohen , Emanuel Gull , David R. Reichman , Andrew J. Millis