Wednesday Afternoon

New Approaches to Long-Range Electron Correlations: In Honor of Mel Levy and John P. Perdew

Viktor Staroverov, *Presiding*

1:30 (315). Stochastic adventures in density functional theory and beyond. **R.R. Baer**, E. Arnon, Y. Cytter, M. Fabian, B. Schpiro, V. Vlcek, E. Rabani, D. Neuhauser
2:00 (316). The strongly constrained and appropriately normed meta-generalized gradient approximation. **J. Sun**
2:30 (317). Fully non-local exchange-correlation functionals from the mathematical structure of the strong-coupling limit of DFT. **P. Gori-Giorgi**, S. Vuckovic
3:00 (318). Temperature and the strong-interaction limit of density functional theory. **A. Pribram-Jones**
3:15 Intermission.
3:30 (319). Electron density errors in approximate density functional calculations. **G.I. Csonka**, P. Mezei
4:00 (320). Orbital-dependent improvements to density-functional approximations: Application to highly charged molecular anions. **M.R. Pederson**, J. Batool
4:30 (321). Dispersion interactions from the exchange-hole dipole moment. **E.R. Johnson**
5:00 (322). Noncollinear spins in density functional theory: Ground state formulation, linear response, stability and single particle excited states. **G. Scalmani**, F. Egidi, X. Li, M.J. Frisch
5:15 (323). DFT functional calibration from highly-accurate energies and densities at different correlation regimes. **E. Matito**
5:30 (324). Density functional theory for spectroscopy and thermochemistry. **M. Biczysko**

Thursday Morning

Orbital Energies, Potentials, and other Kohn-Sham properties: In Honor of Mel Levy and John P. Perdew

Weitao Yang, *Presiding*

9:00 (596). Modeling the shifted Hartree-exchange-correlation potential in direct energy Kohn-Sham theory. **D. Tozer**, M.P. Levy, D. Sharpe
9:30 (597). Exact exchange-correlation potentials of two-electron systems and exact Fermi potentials. **V.N. Staroverov**, I.G. Ryabinkin, E. Ospadov
10:00 (598). Directly patching exchange-correlation energy in density functional theory. **C. Huang**
10:15 Intermission.
10:30 (599). Making high accuracy affordable through DFT. **G.A. Petersson**
10:45 (600). Unraveling the electronic structure of organic photovoltaic donors: Selecting density functionals through electron paramagnetic resonance parameter prediction. **K. Mardis**, J. Niklas, O. Poluektov, C. Mallares, K. Wallace

Thursday Morning (Continued)

11:00 (601). Influence of intramolecular and intermolecular interactions on the sensitivity of energetic materials. **A.L. Shoaf**, C.A. Bayse
11:15 (602). Towards an Ab initio understanding of the hydrated electron: DFT-based molecular dynamics simulations of water anion clusters. C. Zho, **B.J. Schwartz**
11:30 (603). Modeling phase equilibria using CP2K software suite. **H. Goel**, N. Rai
11:45 (604). Utilizing advanced kinetic energy density based ingredients for novel local hybrid mixing functions. **J.W. Furness**, J. Sun
12:00 (605). Multireference density functional theory with generalized auxiliary systems for ground and excited states. **Z. Chen**, D. Zhang, Y. Jin, Y. Yang, N. Su, W. Yang

Thursday Afternoon

Conceptual Tools and Related Applications: In Honor of Mel Levy and John P. Perdew

Jose Luis Gazquez, *Presiding*

1:30 (634). Density based electron localization function. **A.E. Mattsson**
2:00 (635). From chemical information in semilocal functionals to correcting a functional. **J. Contreras-Garcia**
2:30 (636). Incorporating charge transfer directionality in a global and local charge transfer model. **A. Vela**, U. Orozco-Valencia, J.L. Gazquez
2:45 (637). The parabolic interpolation is justified by thermodynamics. **M. Franco-Pérez**, J.L. Gazquez, P. Ayers, A. Vela
3:00 (638). Conceptual DFT formulated general purpose reactivity indicator for predicting and classifying the reactivity of sites within a molecule. **J.S. Anderson**, P. Ayers
3:15 (639). Maximum hardness principle applied for solids: Systems, reactions, phenomena. **W. Grochala**
3:30 (640). Chemical transferability of functional groups follows from the nearsightedness of electronic matter. **S. Fias**, P.F. Geerlings, P. Ayers
3:45 Intermission.
4:00 (641). Variational information-theoretic atoms-in-molecules. **F. Heidar-Zadeh**, T. Verstraelen, E. Vohringer-Martinez, P. Bultinck, P. Ayers
4:30 (642). Theory and applications of density-base energy decomposition analysis (DEDA). **Q. Wu**
4:45 (643). Frustrated Lewis trios and long-range hole interactions. **J. Echeverria**
5:00 (644). Benchmarking density functional methods for calculation of state energies of first row spin-crossover molecules. **J. Cirera Fernandez**, E. Ruiz
5:15 (645). Systematic determination of Hubbard *U* for high-throughput DFT calculations. **J.W. Bennett**, S. Spurgeon, I. Metz, B. Hudson, S.E. Mason
5:30 (646). Simulating ionization-triggered attosecond charge migration with TDDFT. A. Bruner, A. Sissay, S. Hernandez, F. Mauger, P. Abanador, M. Gaarde, K. Schafer, **K. Lopata**

ACS DIVISION OF PHYSICAL CHEMISTRY

Adventures in Density Functional Theory:

A Symposium in Honor of Mel Levy and John Perdew

Paul Ayers
Weitao Yang
Organizers

Morial Convention Center
Room 219

March 18-22, 2018

Cosponsored by COMP

Sunday Morning
In Memory of Robert G. Parr: The Early Years
Mel Levy, *Presiding*

8:30 (1). Atoms and bonds in molecular electronic wave functions: An intrinsic analysis. **K. Ruedenberg**
8:50 (2). Summation by educated match: A new, powerful technique to sum divergent series. G. Álvarez, **H.J. Silverstone**
9:10 (3). Solving the Schrödinger equation of atoms and molecules with the free complement theory. **H. Nakatsuji**
9:30 (4). Chemical potential, chemical hardness, Fukui function and dual descriptor for interacting systems. **J.L. Gazquez**, M. Franco-Perez, A. Vela
9:50 Intermission.
10:10 (5). Charge-separation models from the fragment-Hamiltonian approach. **S. Valone**
10:30 (6). Density functional theory in parameter space and its application to dynamics in condensed phase. **S. Ghosh**
10:50 (7). Thermodynamical representation of density functional theory. **A. Nagy**
11:10 (8). Localized orbital scaling correction for systematic elimination of delocalization error in density functional approximations. **W. Yang**

Sunday Afternoon
In Memory of Robert G. Parr: The Later Years
John Perdew, *Presiding*

1:30 (42). On the nature of the real part of the electron density and the resulting Fukui functions obtained from complex wave functions of temporary anion states. **R.C. Morrison**
1:50 (43). Renewed energy density concept as quantum mechanics 100 years of mystery is solved. **A. Tachibana**
2:10 (44). Pauli principle and the confinement of electron pairs In A symmetric double well potential. **P. Fuentealba**, T. Novoa, C. Cardenas
2:30 (45). Fluxional behavior and noble gas binding ability of boron clusters. **P. Chattaraj**
2:50 Intermission.
3:10 (46). The CsI band gap under strong compression. **A. Cedillo**
3:30 (47). Conceptual density functional theory: Applications in bonding, chemical reactivity and molecular design. **F.J. De Proft**
3:50 (48). Functional derivatives and differentiability in density-functional theory. **Y.A. Wang**
4:10 (49). Density functional reactivity theory: Its recent developments and applications. **S. Liu**

Monday Morning
Fundamental Advances and New Directions in Density Functional Theory: In Honor of Mel Levy and John P. Perdew
Michael Herman, *Presiding*

8:30 (93). On variational principles, and exact functional constraints, for ground states and excited states in time-independent density functional theory. **M.P. Levy**
9:00 (94). Adventures in density functional theory by a wavefunction theorist: A different, powerful perspective. **R. Bartlett**, D.S. Ranasinghe, Y. Park, P. Verma, Y. Jin, A. Perera
9:30 (95). Active space dependence of energy components and ingredients in multiconfiguration pair-density functional theory. **P. Sharma**, D.G. Truhlar, L. Gagliardi
9:45 Intermission.
10:00 (96). What Bob Parr has wrought: Quantum mechanics based reaction mechanisms for electrocatalysis. **W.A. Goddard**
10:30 (97). Where's my oscillator strength? **D.N. Beratan**
11:00 (98). Advances in orbital-free density functional theory simulations of materials. B. Gonzalez del Rio, W.C. Witt, J.M. Dieterich, **E.A. Carter**
11:30 (99). Nonlocal kinetic energy functionals by functional integration. **W. Mi**, A. Genova, M. Pavanello

Monday Afternoon
Random Phase Approximation and Excited States: In Honor of Mel Levy and John P. Perdew
Eberhard Gross, *Presiding*

1:30 (142). Optimized power series approximation for the correlation kernel for highly accurate and generally applicable Kohn-Sham methods based on the adiabatic-connection fluctuation dissipation theorem. **A. Goerling**, J. Erhard
2:00 (143). Following the path of Mel and John into the time-domain. **N.T. Maitra**
2:30 (144). Many body techniques for surface energies, interlayer binding energies and structural phase transitions. **A. Ruzsinszky**
3:00 (145). Generalized optimized effective potential for orbital functionals and self-consistent calculation of random phase approximations. **Y. Jin**, D. Zhang, Z. Chen, N. Su, W. Yang
3:15 Intermission.
3:30 (146). Single-particle excitation energies from the virial theorem. **A.D. Becke**
4:00 (147). Dreaming of banishing exact exchange: Semi local functionals as a key to understanding natural light harvesting? **S. Kuemmel**, T. Aschebrock, I. Schelter, T. de Queiroz
4:30 (148). Weight dependence of the exchange-correlation energy in ensemble density-functional theory. **E. Fromager**
4:45 (149). Reference determinant dependence of the random phase approximation in 3d transition metal chemistry. **J.E. Bates**, P. Mezei, G.I. Csonka, J. Sun, A. Ruzsinszky
5:00 (150). Improving the accuracy of inner shell excitation energies and reducing the self-interaction error with ionization potential optimized global hybrid functional. **Y. Jin**, R.J. Bartlett
5:15 (151). An introduction to projection functional theory: A method for finding excited states. **D.A. Engebretson**
5:30 (152). Low-lying excited states by constrained DFT. **P. Ramos**, M. Pavanello

Tuesday Morning
Developing New Density Functionals: In Honor of Mel Levy and John P. Perdew
Paul Ayers, *Presiding*

8:30 (213). SCAN density functional: Predictive power of 17 exact constraints. **J.P. Perdew**
9:00 (214). Structural and ferroelectric properties of prototypical ferroelectric materials: Comparative first-principles investigations. **Y. Zhang**, J. Sun, J.P. Perdew, X. Wu
9:15 (215). New semilocal density functional and its performance. **J. Tao**
9:45 (216). The correlation factor model: Generalizations and applications. **M. Ernzerhof**
10:15 Intermission.
10:30 (217). Recent advances in density functional theories. **D.G. Truhlar**
11:00 (218). Combinatorial design and assessment of a new double hybrid density functional. N. Mardirossian, **M.P. Head-Gordon**
11:30 (219). Interrogating the "B05" density functional for non-locality information. **S.G. Dale**, E.R. Johnson, A.D. Becke

Wednesday Morning
New Approaches to Long-Range Electron Correlations: In Honor of Mel Levy and John P. Perdew
Paola Gori-Giorg, *Presiding*

8:30 (267). Exact factorization of the N-electron wave function and its relation to density functional theory. **E. Gross**
9:00 (268). Constrained searches in density functional and wavefunction theories. **A.J. Cohen**, P. Mori-Sanchez
9:30 (269). Electron densities (still) in search of Hamiltonians. **S.R. Atlas**
10:00 Intermission.
10:15 (270). Importance of theory in density functional theory. **K. Burke**
10:45 (271). Calculating the Levy constrained search for the exact functional of density functional theory. **P. Mori-Sanchez**, A.J. Cohen
11:15 (272). Describing discontinuity in exchange-correlation functional and strong correlation with fractional-spin correction. **N. Su**, C. Li, W. Yang
11:30 (273). Systematic improvement of approximations with smooth Coulomb potentials. **C.E. Gonzalez**, T. Verstraelen, P. Ayers, A. Savin