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
5:00 (2). Summation by educated match: A new, powerful technique to sum  
divergent series. G. Alvarez, H.J. Silverstone
9:10 (3). Solving the Schrödinger equation of atoms and molecules with the free  
complement theory. H. Nakatsui
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 Intermision.
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

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 Intermision.
10:00 (96). What Bob Parr has wrought: Quantum mechanics based mechanism  
electrochemistry. 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. Goering, 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
3:30 Intermision.
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.J. Csaszar, 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
states. D.A. Engebritson
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
9:45 (216). The correlation factor model: Generalizations and applications.  
M. Ernzerhof
10:15 Intermision.
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-Giorgi, 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
10:00 Intermision.
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. Verstraeten, P. Ayers, A. Savin

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). Paul principle and the confinement of electron pairs in A symmetric  
double well potential. P. Fuentealba, T. Nova, C. Cardenas
2:30 (45). Fluxional behavior and noble gas binding ability of boron clusters.  
P. Chattaraj
2:50 Intermision.
3:10 (46). The Csl 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
Y.A. Wang
S. Liu