Sixteenth Annual Workshop on Recent Developments in Electronic Structure Methods (ES2004)

Rutgers, The State University of New Jersey
New Brunswick, NJ, USA
May 27 - 30, 2004

Schedule of Events

Thursday, May 27

5:00 - 9:00 pm  DORM CHECK-IN  (Stonier Hall - Dorm residents only)
6:00 - 9:00 pm  RECEPTION  (Zimmerli Art Museum)

Friday, May 28

7:30 - 8:15 am  BREAKFAST SERVED  (Brower Commons - Dorm residents only)
8:15 - 8:50 am  REGISTRATION  (Voorhees Hall)

SCIENTIFIC PROGRAM  (Voorhees Hall)

8:50 - 9:00 am  WELCOMING REMARKS
Holly Smith, Executive Dean, Faculty of Arts and Sciences

Session Chair: John Wilkins

9:00 - 9:35 am  John P. Perdew, Tulane University
Meta-Generalized Gradient Approximation: Third Rung on the Ladder of Density Functional Approximations

9:35 - 10:10 am  Weitao Yang, Duke University
Potential Functionals: Solution to the v-representability Problem and Theoretical Foundation for the Optimized Effective Potential in Density Functional Theory

10:10 - 10:30 am  COFFEE BREAK

Session Chair: Hardy Gross

10:30 - 11:05 am  Kiril Tsemekhman, University of Washington
Self-Consistent Implementation of Self-Interaction Corrected Density Functional Theory to Confined and Extended Systems

11:05 - 11:40 am  David C. Langreth, Rutgers University
Van der Waals Density Functional Theory with Applications
11:40 - 12:15 pm  Morrel H. Cohen, Rutgers University
*Interpreting the Kohn-Sham Spectrum*

12:30 - 1:15 pm  LUNCH SERVED  *(Brower Commons)*

**Session Chair: John Tully**

1:45 - 2:20 pm  Hong Guo, McGill University
*Modeling Charge Transport in Molecular Electronics: a Combined DFT and Non-equilibrium Green's Function Approach*

2:20 - 2:55 pm  Jeffrey B. Neaton, LBNL and U.C. Berkeley
*First-principles Studies of Electron Transport through Nanostructures and Molecules Using a Scattering State Approach*

3:05 - 4:35 pm  POSTER SESSION I

4:35 - 5:10 pm  Giulia Galli, Lawrence Livermore National Laboratory
*First Principles Simulations of Water and Simple Aqueous Solutions*

5:10 - 5:45 pm  Nikos L. Doltsinis, Ruhr-Universitaet Bochum
*Nonadiabatic Ab-initio Molecular Dynamics for High-dimensional Systems*

[ DINNER ON YOUR OWN IN NEW BRUNSWICK ]

**Saturday, May 29**

7:30 - 8:15 am  BREAKFAST SERVED  *(Brower Commons - Dorm residents only)*

**SCIENTIFIC PROGRAM**  *(Voorhees Hall)*

**Session Chair: Mei-Yin Chou**

9:00 - 9:35 am  Claudia Filippi, University of Leiden
*Ground and Excited-state QMC Energies: The Importance of Wave Function Optimization*

9:35 - 10:10 am  Lubos Mitas, North Carolina State University
*Coupled Quantum Monte Carlo and Ab-Initio Molecular Dynamics Simulations*

10:10 - 10:30 am  COFFEE BREAK

**Session Chair: Cyrus Umrigar**

10:30 - 11:05 am  Henry Krakauer, College of William and Mary
*Quantum Monte Carlo Method for Real Materials: Random Walks in Slater Determinant Space*

11:05 - 11:40 am  T. Daniel Crawford, Virginia Tech
Local Correlation in Molecular Response Properties

11:40 - 12:15 pm  Catalin Spataru, U.C. Berkeley
Non-equilibrium Quasiparticle Spectrum of Highly IrradiatedSemiconductors

12:30 - 1:15 pm  LUNCH SERVED  (Brower Commons)

Session Chair: Jerry Bernholc

1:45 - 2:20 pm  Sergej Y. Savrasov, New Jersey Institute of Technology
Electronic Structure Calculations with Dynamical Mean Field Theory

2:20 - 2:55 pm  Peter D. Haynes, University of Cambridge
Linear-scaling Density-functional Theory with Plane Waves

3:05 - 4:35 pm  POSTER SESSION II

4:35 - 5:10 pm  Donald R. Hamann, Rutgers University and Lucent Bell Laboratories
Strain Perturbations and Other Recent Developments in the ABINIT Software Package

5:10 - 5:45 pm  Stefan Goedecker, University of Basel
Structure Determination of Large Systems: Finding Local and Global Minima of the Potential Energy Surface

8:00 pm  CONFERENCE BANQUET  (Soho on George)

Sunday, May 30

7:30 - 8:15 am  BREAKFAST SERVED  (Brower Commons - Dorm residents only)

SCIENTIFIC PROGRAM  (Voorhees Hall)

Session Chair: Nicola Marzari

9:00 - 9:35 am  Serge M. Nakhmanson, North Carolina State University
Design of New Ferroelectric Polymers through Computer Simulations

9:35 - 10:10 am  Bernard Kirtman, U.C. Santa Barbara
Calculation of Nonlinear Optical Properties of Conjugated Molecules and Polymers

10:10 - 10:20 am  Richard M. Martin, University of Illinois
Brief Introduction to New Textbook and Resources under Construction

10:20 - 10:40 am  COFFEE BREAK

Session Chair: Don Hamann

10:40 - 11:15 am  Michelle D. Johannes, Naval Research Laboratories
Can Electronic Structure Calculations Explain the Complex Properties of Na$_2$CoO$_2$?

11:15 - 11:50 am  Eberhard K.U. Gross, Freie Universitat Berlin
Density Functional Theory of Superconductivity

11:50 - 12:00 pm  CONCLUDING REMARKS

12:15 - 1:00 pm  LUNCH SERVED  (Brower Commons)

12:45 - 2:15 pm  DORM CHECK-OUT  (Stonier Hall - Dorm residents only)

END

I2. Kudin, K.N., Car, R., and Resta, R. *Longitudinal Polarizability of Long Polymeric Chains: Quasi-One-Dimensional Electrostatics as the Origin of Slow Convergence*

I3. Thygesen, K.S., Hansen, L.B., and Jacobson, K.W. *Partly Occupied Wannier Functions*

I4. Swalina, C., Pak, M.V., and Hammes-Schiffer, S. *Application of the Nuclear-Electronic Orbital (NEO) Method to Proton Transfer Reactions: Electron-Proton Correlation Effects*


I8. Whittingham, T., and Burke, K. *Correlation Energies in the High Density Limit*


I11. Bagayoko, D. *A Mathematical Solution to the Band Gap Catastrophe*


I17. Zhao, Q., Nardelli, M.B., Lu, W., and Bernholc, J. Carbon Nanotube-Metal Cluster Composites: A new Road to Chemical Sensors?

I18. He, L., Bester, G., and Zunger, A. Metal-Nonmetal Transition and Excitonic Ground State in InAs/InSb Quantum Dots


I20. Güçlü, A.D., and Umrigar, C.J. Quantum Monte Carlo Study of Planar Quantum Dots in Magnetic Fields


I23. Wang, X., and Car, R. Pseudopotential and Plane-Wave Base TPSS Meta-GGA, and Application to the Melting of Silicon


I27. Trinkle, D.R. The Lattice Green Function for Phonons: Decoupling Short and Long Range Contributions


I29. Lechermann, F., Biermann, S., and Georges, A. Electronic Correlations in the Multi-Orbital System BaVS$_3$
I30. Park, K., Baruah, T., Bernstein, N., Richardson, S.L., and Pederson, M.R. *Study of Magnetic Anisotropy and Tunneling in Molecular Magnets using Density Functional Theory*

I31. Hazzard, K.R.A., Kim, J., and Wilkins, J.W. *Electronic Charge Distribution of Silicon Tri-Interstitial Defects*

I32. Íñiguez, J., and Yildirim, T. *Interplay Between Structure and Magnetism in Se$_{1-x}$Te$_x$CuO$_3$ Alloys*

I33. Nunez, M., and Nardelli, M.B. *Properties of Interfaces Between metals and High-K Dielectrics*

I34. Tang, P., and Holzwarth, N.A.W. *Comparison of the Electronic Structures of Three Phases of FePO$_4$ (Olivine, Quartz, and CrVO$_4$)*
II1. Tulip, P.R., Clark, S.J., and Refson, K. Implementation of a Density Functional Perturbation Theory Algorithm within a Plane Wave Ab Initio Code


II3. Chu, J-W., Brooks, B.R., and Trout, B.L. A Super-Linear Minimization Scheme for the Nudged Elastic Band Method


II5. Iddir, H., Ogut, S., Disko, M.M., and Browning, N.D. Theoretical and Experimental Studies of Pt and Au on TiO₂ Surfaces


II8. Wasserman, A., Maitra, N.T., and Burke, K. Electron-Ion Scattering from Time-Dependent Density Functional Theory

II9. Zhang, F., Maitra, N.T., Cave, R.J., and Burke, K. Nearly Degenerate Excitations in Density Functional Theory

II10. Gaudoin, R., and Burke, K. Density Functional Theory, Adiabatic Connection, and Excited States

II11. Gibson M.C., Clark, S.J., and Brand, S. Non-Local Treatment of Correlation in Density Functional Theory


II13. Armiento, R., and Mattsson, A. Recent Developments of Subsystem Functionals

II15. Kozhushner, M.A., Posvyanskii, V.S., and Oleynik, I.I. Bound States of Tunneling Electrons in Molecular Wires

II16. Yang, L., Chou, M.Y., and Zhao, X.Y. Lattice Vibrations of Silicon Nanowire [110]


II18. Andersen, K.E., Kumar, V., Kawazoe, Y., and Pickett, W.E. Origin of Permanent Electric Dipoles in Homonuclear Nb\(_n\) Clusters


II22. Lenosky, T.J., Hennig, R.G., Wilkins, J.W., Trinkle, D.R., Woodward, C., and Rudin, S. Ab-Initio Based Classical Potential for Molybdenum Describes Motion of Screw and Edge Dislocations in BCC Molybdenum

II23. Sit, P.H.-L., Cococcioni, M, and Marzari, N. Liquid Water, Solvated Ions, and Electron-Transfer Reorganization Energies from First-Principles Molecular Dynamics

II24. Welch, E.N., Hazzard, K.R.A, and Wilkins, J.W. Free Energy and Transition Rate Calculations Beyond the Harmonic Approximation


II27. Shi, L., and Papaconstantopoulos, D.A. Harrison’s Tight-Binding Theory Revisited


II29. Ku, W., Vogt, T., Davenport, J., and Volja, D. Theoretical Study of Magnetic Orbital and Lattice Structure of MnF\(_3\)


II31. Umari, P., and Pasquarello, A. Hyper-Raman Spectra of Vitreous Silica from First Principles
II32. Idrobo, J.C., Ogut, S., Yildirim, T., Klie, R.F., and Browning, N.D. The Electronic and Superconducting Properties of Oxygen-Ordered MgB$_2$ Compounds of the Form Mg$_2$B$_3$O$_x$

II33. Ederer, C., and Spaldin, N.A. First-Principles Prediction of Magnetoelectric Switching in BiFeO$_3$