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 Irradiated Semiconductors

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_xCoO_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

Poster session I

Friday, May 28, 3:05 - 4:35 pm

I1. Abraham, Y., Rojas, M., Holzwarth, N.A.W., and Plemmons, R. *Optimization with Surrogates for Electronic-Structure Calculations*

I2. Kudin, K.N., Car, R., and Resta, R. *Longitudal 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*

I5. Rohlfing, M., Wang, N.-P., Kruger, P., and Pollmann, J. *Dynamics of Excited Electronic States*

I6. Zhang, Q., and Lewis, S.P. *Weak Bonding of Corner Carbon Atoms in Titanium-Carbide Nanocrystals*

I7. Takeuchi, N., Kanai, Y., and Selloni, A. *Reaction of Alkynes with H-Si(111): A Density Functional Theory Study*

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

I9. Atlas, S.R., and Valone, S.M. *Ensemble Density Functional Theory for Multiscale Dynamical Potentials*

I10. Abraham, Y., and Holzwarth, N.A.W. *A Method for Calculating Surface Electronic Structures Using Semi-Infinite Boundary Conditions*

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

I12. Csonka, G.I., Ruzsinsky, A., Tao, J., and Perdew, J.P. *Energies of Organic Molecules and Atoms in Density Functional Theory*

I13. Kanai, Y., Wang, X., Tilocca, A., Selloni, A., and Car. R. *First-Principles String Molecular Dynamics for Finding Chemical Reaction Pathways*

I14. George, A.M., Santiso, E., Gibbons, K.E., and Nardelli, M.B. *Dissociation of Formaldehyde in Nanostructured Carbon Materials*

I15. Lee, Y-S., Nardelli, M.B., and Marzari, N. *"On-the-Fly" Electronic Structure and Quantum Conductance of nanostructures from Maximally-Localized Wannier Functions: The Case of Functionalized Carbon Nanotubes*

I16. Tchernatinsky, A., Sumanasekera, G., Wu, S.Y., and Jayanthi, C.S. *A First-Principles Calculation of Potassium-Covered Carbon Nanotubes and Other Related Structures*

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*

I19. Das, D., Martin, R.M., Kim, J., Zhang, L., and Lebuton, J-P *QMC Calculation of a Realistic Double Quantum Dot Using a Stochastic Poisson Solver*

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

I21. Hennig, R.G., Umrigar, C.J., and Wilkins, J.W. *Diffusion Monte Carlo for High-Pressure Silicon Phases*

I22. Wood, B., and Marzari, N. *A First-Principles Study of Ionic Conductivity in Superionic Solids*

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

I24. Scherlis, D., and Marzari, N. Π-*Stacking in Thiophene Oligomers as the Driving Force for Novel Electroactive Materials and Devices*

I25. D'Avezac, M., Marzari, N., and Mauri, F. *First-Principles NMR in Metallic Systems: All-Electron Magnetic Response for the Chemical and Knight Shifts from Pseudopotential Calculations*

I26. Carrier, P., and Wei S-H. *A Calculated Spin-Orbit Splitting of All Diamond-Like and Zinc-Blende Semiconductors: Effects of $p_{\frac{1}{2}}$ Local Orbitals and Chemical Trends*

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

I28. Peles, A., Alford, J.A., Ma, Z., Yang, L., and Chou, M.Y. *First-Principles Study of $NaAlH_4$ and Na_3AlH_6 Complex Hydrides*

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* $Se_{1-x}Te_xCuO_3$ *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* $CrVO_4$*)*

Poster session II

Saturday, May 29, 3:05 - 4:35 pm

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*

II2. Torsti, T., Ignatius, J., Puska, M.J., and Nieminen, R.M. *Multigrid Methods for Electronic Structure Calculations*

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

II4. Karcz, J.S., and Chernoff, D.F. *Finding Occupancies Through Direct Minimization of the Free Energy in Density-Functional Calculations*

II5. Iddir, H., Ogut, S., Disko, M.M., and Browning, N.D. *Theoretical and Experimental Studies of Pt and Au on TiO_2 Surfaces*

II6. Li, X., Schlegel, H.B., Frisch, M.J., and Tully, J.C. *Time-Dependent Density Functional Theory for Studying the Energies and Lifetimes of Excited Adsorbate States on Metal Surfaces*

II7. Tilocca, A., and Selloni, A. *Multilayer Water on Anatase (101) Surface: Adsorption Modes and Reactivity*

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*

II12. Dion, M., Rydberg, H., Schroder, E., Hyldgaard, P., Langreth, D.C., and Lundqvist, B.I. *Van der Waals Forces in Density Functional Theory*

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

II14. Zhao, X., and Chou, M.-Y. *First-Principles Study of Semiconductor Nanowires: Electronic and Optical Properties*

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]*

II17. Prendergast, D., Grossman, J.C., Williamson, A.J., Fattebert, J-L., and Galli, G. *Optical Properties of Silicon Nanoparticles in the Presence of Water*

II18. Andersen, K.E., Kumar, V., Kawazoe, Y., and Pickett, W.E. *Origin of Permanent Electric Dipoles in Homonuclear Nb_n Clusters*

II19. Chiesa, S., Ceperley, D.M., and Zhang, S. *A New Estimator for Nuclear Forces in Quantum Monte Carlo*

II20. Esler, K.P., and Ceperley, D.M. *PIMC for Heavy Atoms with Pseudo-Hamiltonians*

II21. Cancio, A., and Chou, M-Y. *Laplacian-Based Model of the Adiabatic Exchange-Correlation Energy Density in Si Crystal and Atom*

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*

II25. Cococcioni, M., Mauri, F., Ceder, G., and Marzari, N. *Electronic-Enthalpy Functional for First-principles Simulations of Finite Systems Under Pressure*

II26. Romero, N.A., Kim, J., and Martin, R.M. *C_{28}-Derived Molecular Solids: Structure, Electron-Phonon Interaction and Doping*

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

II28. Junquera, J., García, A., Verstraete, M., *A New Proposal for a Unified Pseudopotential Format*

II29. Ku, W., Vogt, T., Davenport, J., and Volja, D. *Theoretical Study of Magnetic Orbital and Lattice Structure of MnF_3*

II30. Du, Y., Hazzard, K.R.A., Hennig, R.G., and Wilkins, J.W. *Fast Diffusion Mechanism of Silicon Tri-Interstitial Defects*

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 $Mg_2B_3O_x$*

II33. Ederer, C., and Spaldin, N.A. *First-Principles Prediction of Magnetoelectric Switching in $BiFeO_3$*