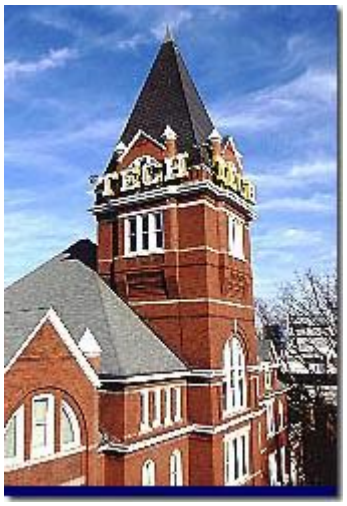
Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods

May 19 - 22, 2000
Web: http://www.physics.gatech.edu/es2000
E-mail: es2000@physics.gatech.edu

new **Important Information for Participants**



Georgia Institute of Technology
Atlanta, Georgia, USA

GENERAL INFORMATION

The Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods (ES2000) will be held at the Georgia Institute of Technology in Atlanta on May 19-22, 2000. This workshop brings together active participants in electronic structure theory from universities, colleges, government labs, and industrial labs around the world. The invited presentations and contributed posters will describe new methods for computing previously inaccessible properties, breakthroughs in computational efficiency and accuracy, and novel applications of these approaches to the study of molecules, liquids, and solids. This conference represents a valuable opportunity for students, postdocs, and senior researchers alike to explain their ideas and learn from each other.

TOP

CONFERENCE ORGANIZATIONS

Local Organizing Committee

Mei-Yin Chou, School of Physics, Georgia Tech
Uzi Landman, School of Physics, Georgia Tech
C. David Sherrill, School of Chemistry, Georgia Tech
Xiao-Qian Wang, CTSPS, Clark Atlanta University

Steering Committee:

Douglas Allan (Corning)
Jerzy Bernholc (North Carolina State University)
Roberto Car (Princeton University)
David Ceperley (University of Illinois)
James Chelikowsky (University of Minnesota)
James Gubernatis (Los Alamos)
Duane Johnson (University of Illinois)
Steven Lewis (University of Georgia)
Steven Louie (UC Berkeley)
Richard Martin (University of Illinois)
Andrew Rappe (University of Pennsylvania)
Mark Stiles (NIST)
Cyrus Umrigar (Cornell University)
David Vanderbilt (Rutgers University)
John Wilkins (Ohio State University)

Sponsors:

School of Physics, Georgia Tech
College of Sciences, Georgia Tech
CTSPS, Clark Atlanta University

TOP

IMPORTANT DATES

March 10 -Suggestions for speakers or lecture topics

May 3 -Registration deadline--without late fee
- Inclusion of poster title in the printed program
- Last day to guarantee dormitory space

May 8 - Deadline for requesting a refund

TOP

PROGRAM

The ES2000 workshop will be held in the Auditorium of the Smithgall Student Services Building on the Georgia Tech campus. (map here) The workshop will begin with a reception on Friday evening, May 19. There will be full days of lectures and poster sessions on Saturday and Sunday, May 20-21, and a half day of lectures on Monday, May 22. Lecturers will be selected by the steering committee at the 2000 APS March Meeting in Minneapolis and invited shortly thereafter. Specific suggestions for speakers or lecture topics are welcome and should be directed to the conference email address no later than March 10, 2000. The poster sessions are an important part of the conference and all attendees are encouraged to participate. If you are planning to present a poster, please send a title and an abstract to the organizing committee by May 3 in order to be included in the printed program.

Possible topics to be presented at ES2000 include density functional theory, quantum Monte Carlo, linear scaling methods, quantum chemistry methods, pseudopotentials,

quantum dynamics, parallel computing, novel basis sets, Car-Parrinello methods, and new applications to physical phenomena.

new **Tentative Schedule of Events** TOP

REGISTRATION

We ask all participants to register on-line prior to the workshop. The registration fee is $215 ($165 for students) if received before May 3, 2000. Post-deadline registrations will incur an additional $50 charge. The modest registration fee includes three nights of single-room apartment-style dormitory lodging, a banquet and all other meals (except one dinner). Participants registering after May 3 cannot be guaranteed dormitory lodging. Refunds can be issued (less an administrative fee of $30) only if a request for cancellation is received in writing by May 8.

Online Registration Form **Credit Card Authorization Form**

TOP

ACCOMMODATIONS

Participants will stay at the Hemphill Avenue Apartments at 900 Hemphill Avenue on the Georgia Tech campus, at the corner of Hemphill and 9th Street (see map). It is within walking distance from the conference site (the Smithgall Student Services building) and is one of the apartment-style residences constructed as part of the 1996 Olympic Village. The Housing staff will provide on-site check-in assistance from 4:30 pm to 8:30 pm on Friday, May 19, 2000. Keys can be picked up from the nearby Conference Housing Office before or after this period. Individuals arriving after midnight will be instructed on how to page the staff to check them into their rooms.

The Hemphill Avenue Apartments are comprised of four-bedroom suite apartments. The units feature kitchens, furnished living rooms, private single bedrooms, and semi-private bathrooms. Kitchenettes feature a refrigerator, microwave, stove, and dishwasher. Kitchen utensils are not provided. A small campus market is available to conference guests and is located adjacent to the apartments. Laundry facilities and exercise room are also available at the complex. Pillow, blanket and linen packet will be provided upon arrival. Towel exchange will be scheduled. The apartment will have basic toiletries including soap, toilet paper, hangers and drinking cups. There is a phone in each apartment suite with free local service. Long distance is available with personal calling card. Television, wake-up calls, or alarm clocks are not provided in the suite. Please plan accordingly.

Each participant will have key access to the individual bedroom as well as the suite and the building, an added security bonus. Parking is available in several lots adjacent to the complex and parking passes will be made available at on-campus housing registration. Additional information regarding on-campus housing and other campus services is available on the Web at http://www.conference.gatech.edu.

Participants preferring to stay at a local hotel are responsible for making their own reservations. Special rates are being offered at the following hotels for ES2000 Workshop guests. You need to CALL THE HOTEL DIRECTLY and mention "ES2000 Workshop" of Georgia Tech. They are all served by Atlanta Airport Shuttle.

Holiday Inn Express - North Avenue
244 North Avenue N.W.
Atlanta, Georgia 30313
(404) 881-0881

It is just across the street from the campus, at the corner of North Avenue and Luckie Street on the south side. Twelve rooms are being held at $79 per night until May 5, 2000. Complimentary extended continental breakfast is included. (web site)

Wyndham Garden Hotel
Peachtree and 10th Street, NE
Atlanta, Georgia 30309
(404) 873-4800

A nice hotel in midtown, about 1.5 miles from the campus. Five rooms are being held at $98 per night until May 5, 2000. It is adjacent to Midtown (N4) MARTA station. (web site)

Regency Suites
975 West Peachtree Street at 10th Street
Atlanta, Georgia 30309
(800) 642-3629 or (404) 876-5003

Five rooms are being held at $79 per night until May 5, 2000. About 1.4 miles from the campus. Complimentary deluxe continental breakfast. Adjacent to Midtown (N4) MARTA station.

TOP

TRAVEL INFORMATION

A. Air Travel Directions

Georgia Tech is conveniently located in midtown Atlanta, which is served by Hartsfield International Airport. To go to Georgia Tech from Hartsfield International Airport, you have four options:

1. Rent a car and drive (click here for driving direction)

2. Take a taxi

3. Take an Airport shuttle

Atlanta Airport Shuttle (404-524-3400 or 800-842-2770) is a complete transportation service located in Hartsfield International Airport. It costs $10 to go to midtown hotels, such as Wyndham Garden Hotel. A short taxi ride afterward will take you to the Georgia Tech campus.

4. Ride Atlanta's rail system, MARTA

The Metropolitan Atlanta Rapid Transit Authority (MARTA) is Atlanta's world-renowned

public transit system which has been providing bus and rail service to the City of Atlanta since 1972. You can find the the rail station near the Baggage Claim area at the airport. The fare is $1.50 for a single ride. There are three rail stations close to Georgia Tech. We recommend that you get off at the North Avenue Station (N3 on MARTA map) and take the free Georgia Tech Stinger bus that connects the MARTA station and the campus (MARTA loop). Get off at Ferst and Hemphill (stop 17). The Hemphill Avenue Apartments will be one short block away. The last bus leaves the North Avenue MARTA station at 8:48 pm on Friday. You will need to take a taxi if you arrive later than that.

Alternatively, you can get off the train at the Midtown Station (N4 on MARTA map). To get to the Hemphill Avenue Apartments from the Midtown Station, you should make sure to first get a bus transfer ticket bus when you use the Marta token in the turnstile AT THE AIRPORT STATION. This ticket allows to you use Marta's extensive bus system to get you to Georgia Tech. Once arriving at the Midtown Station you will get on bus route 37. You will get off the bus at the corner of Hemphill Avenue and Tenth Street. The Hemphill Avenue Apartments will be the second building south of the intersection.

Driving directions to the Hemphill Avenue Apartments at Georgia Tech from the Airport

1. Take Interstate 75/85 North to the Georgia Tech/10th Street Exit (Exit 250).
2. At the traffic light, take a left onto 10th Street.
3. Proceed through four stoplights and make a left onto Hemphill Avenue at the fifth light.
4. The Hemphill Avenue Apartment will be the second building on your right at the corner of Hemphill and 9th Street. Make a right onto 9th Street for parking.
5. Parking information can be found here.

TOP

B. Driving Directions

Driving directions to the Hemphill Avenue Apartments at Georgia Tech from North of Atlanta

1. Take Interstate 75 or 85 South to the Techwood Drive/10th/14th Street Exit (Exit 250 on I-75 and Exit 84 on I-85, respectively).
2. Proceed straight through the first traffic light and stay in the central lane (the right lane will be closed for construction).
3. At the traffic light, take a right on 10th Street.
4. Proceed through three stoplights and make a left onto Hemphill Avenue at the fourth light.
5. The Hemphill Avenue Apartment will be the second building on your right at the corner of Hemphill and 9th Street. Make a right onto 9th Street for parking.
6. Parking information can be found here.

TOP

Driving directions to the Hemphill Avenue Apartments at Georgia Tech from South of Atlanta

1. Take Interstate 75/85 North to the Georgia Tech/10th Street Exit (Exit 250).

2. At the traffic light, take a left onto 10th Street.
3. Proceed through four stoplights and make a left onto Hemphill Avenue at the fifth light.
4. The Hemphill Avenue Apartment will be the second building on your right at the corner of Hemphill and 9th Street. Make a right onto 9th Street for parking.
5. Parking information can be found here.

TOP

Driving directions to the Hemphill Avenue Apartments at Georgia Tech from Augusta/East of Atlanta

1. Follow Interstate 20 West until you reach Atlanta.
2. Take Interstate 75/85 North to the Georgia Tech/10th Street Exit (Exit 250).
3. At the traffic light, take a left onto 10th Street.
4. Proceed through four stoplights and make a left onto Hemphill Avenue at the fifth light.
5. The Hemphill Avenue Apartment will be the second building on your right at the corner of Hemphill and 9th Street. Make a right onto 9th Street for parking.
6. Parking information can be found here.

TOP

Driving directions to the Hemphill Avenue Apartments at Georgia Tech from Birmingham/West of Atlanta

1. Follow Interstate 20 East until you reach Atlanta.
2. Take Interstate 75/85 North to the Georgia Tech/10th Street Exit (Exit 250).
3. At the traffic light, take a left onto 10th Street.
4. Proceed through four stoplights and make a left onto Hemphill Avenue at the fifth light.
5. The Hemphill Avenue Apartment will be the second building on your right at the corner of Hemphill and 9th Street. Make a right onto 9th Street for parking.
6. Parking information can be found here.

TOP

Parking at Georgia Tech

ES2000 has secured visitor-parking permits for the participants. These permits will be issued at on-site registration. The permit will allow long-term parking in a designated lot(s). Please use one of the following options before receiving a permit. The permit is needed for Friday and Monday. During the weekends and evenings, most of the parking lots are open.

The campus has over 125 metered spaces conveniently located in both academic and residential areas. The first 15 minutes are free of charge by pressing the button marked on the parking meter. Additional time up to 2 hours may be purchased for $.25 per 15 minutes. In residential areas, the meters will be enforced 24 hours, 7 days per week. Other meter locations will be enforced from 8:00 a.m. to 5:00 p.m.

Visitor Parking lots are located in two locations on campus. The first is located at the southeast corner of Ferst Drive and State Street. The other is adjacent to the Student Center off Ferst Drive. An attendant staffs both lots Monday through Friday from 7:00 a.m. to 7:00

p.m. The attendant at each location will be helpful in providing visitors with information and directions. The cost for visitor parking lots is $.50 per half-hour, with a maximum of $4.00 per day. Users will pay upon exit. See the parking map.

TOP

POSTER SUBMISSION

If you are interested in presenting a poster, please submit a camera-ready abstract, including the title, author(s), and author affiliation(s) by May 3, 2000 to be included in the printed program. After deadline posters are also welcome. The size of the poster boards is 40" x 60".

Please email your abstract to es2000@physics.gatech.edu in one of the following forms: postscript, pdf, Word, or WordPerfect, and include the word "abstract" in the subject line of the message.

TOP

WEATHER INFORMATION

The average temperatures in Atlanta in the month of May are 60-79 Fahenheit/16-26 Celsius. Afternoon thunderstorms are common in summer months, so an umbrella may be needed.

TOP

Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods (ES2000)

May 19 – 22, 2000
Georgia Institute of Technology

Schedule of Events

Friday, May 19

7:00 – 9:00 pm Registration and Reception (Hemphill Avenue Apartments)

Saturday, May 20

7:00 – 8:20 am Breakfast (Woodruff Residence Hall)

8:30 – 8:45 am Welcome and Opening Remarks (Auditorium, Smithgall Student Services)
Dean Gary Schuster, College of Sciences, Georgia Tech

Session I -- Chair: Donald Hamann

8:45 – 9:20 am **Mats Persson**, Chalmers/Göteborg University
Theory of Single Molecule Vibrational Spectroscopy and Microscopy

9:20 – 9:55 am **Christopher Roland**, North Carolina State University
Theoretical Investigations of Quantum Transport through Carbon-Nanotube Devices

9:55 – 10:25 am Morning Break

Session II -- Chair: Eric Shirley

10:25 – 11:00 am **George Bertsch**, University of Washington
Real-Time Implementation of TDDFT

11:00 – 11:35 am **Eric Chang**, University of California at Berkeley
Optical Spectrum and Excitons of Alpha Quartz

11:35 – 1:00 pm Lunch Break

Session III – Chair: Raffaele Resta

1:00 – 1:35 pm **Laurent Bellaiche**, University of Arkansas
Finite Temperature Properties of Ferroelectric Alloys from First Principles

1:35 – 2:10 pm **Bijaya Karki**, University of Minnesota
High-Pressure Thermoelasticity of Minerals from First Principles

2:10 – 3:40 pm Poster Session and Afternoon Break

Session IV – Chair: W. Matthew Foulkes

3:40 – 4:15 pm **Stephen Fahy**, University College, Cork
Optimal Single-Particle Orbitals from Energy Fluctuations in Correlated Wavefunctions

4:15 – 4:50 pm **Burkhard Militzer**, University of Illinois at Urbana-Champaign
Path Integral Simulation of Hot, High Pressure Hydrogen

4:50 – 5:25 pm **Claudia Filippi**, University College, Cork
Computation of Forces in Quantum Monte Carlo

Sunday, May 21

7:15 – 8:35 am Breakfast (Woodruff Residence Hall)

Session V – Chair: David Sherrill

8:45 – 9:20 am **Rodney J. Bartlett**, University of Florida
Ab initio Density Functional Theory

9:20 – 9:55 am **Martin Städele**, University of Illinois at Urbana-Champaign
Density-Functional Calculations with Exact Exchange

9:55 – 10:25 am Morning Break

Session VI – Chair: John Wilkins

10:25 – 11:00 am **Sergej Savrasov**, Rutgers University
Electronic Structure Calculations with Dynamical Mean Field Theory

11:00 – 11:35 am **Mark Jarrell**, University of Cincinnati
Dynamical Cluster Approximation

11:35 – 1:00 pm Lunch Break

Session VII – Chair: Xiao-Qian Wang

1:00 – 1:35 pm **Ursula Röthlisberger**, ETH
Overcoming the Time Scale Problem in Ab Initio Molecular Dynamics Simulations

1:35 – 2:25 pm **Arthur Voter**, Los Alamos National Laboratory
Methods for Accelerating Molecular Dynamics Simulation of Infrequent Events

2:25 – 3:55 pm Poster Session and Afternoon Break

Session VIII – Chair: Steven Lewis

3:55 – 4:30 pm **Julie B. Staunton**, University of Warwick
Spin Fluctuations in Nearly Magnetic Metals from ab-initio Dynamical Spin Susceptibility Calculations

4:30 – 5:05 pm **Leeor Kronik**, University of Minnesota
Electronic and Structural Properties of Sodium Clusters: A Pseudopotential Based Density Functional Approach

6:30 – 9:00 pm Banquet (Student Center Ballroom)

Monday, May 22

7:15 – 8:35 am Breakfast (Woodruff Residence Hall)

Session IV – Chair: Jerry Bernholc

8:45 – 9:20 am **Giulia Galli**, Lawrence Livermore National Laboratory
First Principles Molecular Dynamics Simulations: Successes and Open Problems

9:20 – 9:55 am **Uzi Landman**, Georgia Tech
Small is Different: Large-Scale Simulations for the Nanoscale

9:55 – 10:25 am Morning Break

Session V – Chair: Cyrus Umrigar

10:25 – 11:00 am **Ivo Nuno Souza**, University of Illinois at Urbana-Champaign
Polarization and Localization in Insulators: Generating Function Approach

11:00 – 11:35 am **Sohrab Ismail-Beigi**, Massachusetts Institute of Technology
New Algebraic Formulation of ab initio Calculation: DFT++

11:35 – 11:50 am Announcements and Closing Remarks

11:50 – 1:30 pm Lunch

Adjourn

ES 2000

CONFIRMED SPEAKERS	
Rodney J. Bartlett	Ab initio Density Functional Theory
Laurent Bellaiche	Finite-Temperature Properties of Ferroelectric Alloys from First Principles
George Bertsch	Real-Time Implementation of TDDFT
Eric Chang	Optical Spectrum and Excitons of Alpha Quartz
Stephen Fahy	Optimal Single-Particle Orbitals from Energy Fluctuations in Correlated Wavefunctions
Claudia Filippi	Computation of forces in quantum Monte Carlo
Giulia Galli	First Principles Molecular Dynamics Simulatioins: Successes and Open Problems
Sohrab Ismail-Beigi	New Algebraic Formulation of ab initio Calculation: DFT++
Mark Jarrell	Dynamical Cluster Approximation
Bijaya Karki	High-Pressure Thermoelasticity of Minerals from First-Principles
Leeor Kronik	Electronic and Structural Properties of Sodium Clusters: A Pseudopotential Based Density Functional Approach
Uzi Landman	Small is Different: Large-Scale Simulations for the Nanoscale
Burkhard Militzer	Path Integral Simulation of Hot, High Pressure Hydrogen
Mats Persson	Theory of Single Molecule Vibrational Spectroscopy and Microscopy
Christopher Roland	Theoretical Investigations of Quantum Transport through Carbon-Nanotube Devices
Ursula Rothlisberger	Overcoming the Time Scale Problem in Ab Initio Molecular Dynamics Simulations
Sergej Savrasov	Electronic Structure Calculations with Dynamical Mean Field Theory
Ivo Nuno Souza	Polarization and Localization in Insulators: Generating Function Approach
Martin Staedele	Density-Functional Calculations with Exact Eexchange
Julie B. Staunton	Spin Fluctuations in Nearly Magnetic Metals from Ab-Initio Dynamical Spin Susceptibility Calculations
Arthur Voter	Methods for Accelerating Molecular Dynamics Simulation of Infrequent Events

GO BACK

POSTER ABSTRACTS	
Dominic R. Alfonso *et al.*	Structure of MgO and CaO(100) Surfaces and their Interaction with Representative Metal Adsorbates
Marie-Laure Bocquet *et al.*	Resoulution of the Surface Structure of an Oxide Film on AG(111) from the Interplay between Measured and Calculated STM Images.
Antonio Cancio *et al.*	A Localized Orbital Approach to the Correlation
Leonardo Colletti *et al.*	"Testing Hund's rule in quantum dots through Diffusion Monte Carlo calculations"
Gabor Csanyi *et al.*	Recent Advances in Tensor-Product Representation of Correlation in the Electron Gas
Rodney Dunning *et al.*	PAW Study of the F-center in LiF
Torkel D. Engeness and *et al.*	High Performance, High precision Multiresolution Calculation of Core-Level Shifts
Jean-Juc Fattebert	Dft Localized Grid-Based Orbitals on Parallel Supercomputers
Michèle Fontaine *et al.*	Phase Behavior of Polymer-Supercritical Fluid Mixtures
Ilya Grinberg *et al.*	Accurate Construction of Transition Metal Pseudopotentials
Richard Hennig *et al.*	Application of Density-Matrix Correlation Functional to Transition Metal Impurities
Natalie Holzwarth *et al.*	A Projector Augmented Wave (PAW) Code for Electronic Structure Calculations -- Pwpaw and Atompaw
Yong-Hoon Kim *et al.*	Exact-Exchange-Base Hybrid-Method Investigations of Small Molecules
Yong-Hoon Kim *et al.*	Urbana-OORI: A New Paradigm for the Electronic-Structure Code Development
Ross A. Lippert *et al.*	Software Engineering in Scientific Computation
Wenchang Lu *et al.*	Ab Initio Calculation of Reflectance Anisotropy Spectroscopy of SiC(001) (3 x 2) Surface
Paul Maragakis *et al.*	ACRES: and Efficient Method for First-Principles Electronic Structure Calculations of Complex System
Nicola Marzari *et al.*	Surface Chemistry from Frst-Principles: Dissociative Chemisorption of Cl_2 on Al(111)
Vincent Meunier *et al.*	Electronic Structure of Polychiral Carbon Nanotubes
Mernd Meyer *et*	Design of Novel Ferroelectric Materials via Compositional

al.	Inversion Symmetry Breaking
Eric A. Perpète *et al.*	Large Vibrational Contributions to the Nonlinear Optical Properties of an Isolated Buckminsterfullerene Molecule
Aaron Puzder *et al.*	Monte Carlo Study of the Exchange-Correlation Energy Density in Atomic Silicon
Ioannis Remediakis *et al.*	Ab Initio Structure and Electronic Proprties of Si(100) Using ACRES
David Richie *et al.*	Self-Adaptive Wavelet-Based Electronic Structure Calculations
Christopher L. Rogers *et al.*	Geometric Formulation of Quantum Stress Fields
Daniel Sanchez-Portal *et al.*	Ab Initio Calculations of the Electronic Structure of $Ca_{14}MnBi_{11}$ and $Ba_{14}MnBi_{11}$
Eric Shirley *et al.*	A Model Dielectric Function with Improve Local-Field Effects
Aleksi Soininen *et al.*	Core Hole - Electron Interaction In Inelastic X-Ray Scattering
Ivo Nuno Souza *et al.*	Maximally-localized Wannier Functions in Compressed Molecular Hydrogen
Alan Tackett *et al.*	Calculation of Selected Eigenvalues using a Jacobi-Davidson Solver
Dallas Trinkle *et al.*	Modeling the hcp to omega Phase Transition in Titanium
Eric J. Walter *et al.*	Investigation of Methyl Radicals on the Rh (111) Surface
Tim Wilkens *et al.*	A Quantum Monte Carlo Study of the One-Dimensional Ionic Hubbard Model
Yashar Yourdshahyan *et al.*	Structural Studay of Alkane Thiols Self-Assembled on Au(111) Surface
G. P. Zhang *et al.*	Ab Initio Results for the Valence-Hole Effects in RIXS from cBN
Xinyuan Zhao *et al.*	Tight-Binding Study of Compressed Solid Hydrogen

GO BACK