Part Two

Computing
Conferences Organized
Roster
Invited Lectures
Publications
Editorships
QTP Seminars
QTP Visitors
A Brief History
Erik Deumens, Director
Computer Hardware and Software Activity

One of J.C. Slater’s less-known contributions to the University of Florida was his leadership in obtaining advanced computing systems. QTP’s computing and visualization systems and services are named in recognition of that innovative vision.

The Xena Project
in Parallel Supercomputing

During Summer and Fall 2000, the RS/6000 SP system in the Slater Computing Laboratory was greatly enhanced by the installation of a system of 134 nodes with 66 MHz POWER CPUs, 64 MByte RAM and 1 GByte or more disk; 38 nodes have 128 MByte of RAM and 41 nodes have a 1 GByte local scratch disk. This machine, called Xena, was constructed locally out of a major subsystem of the ex-Maui Supercomputer Center machine plus spares. They were obtained via a competitive Department of Defense award (High Performance Computing Modernization Program).

This machine is denoted phase I (Xena-I) because the strategy of the Xena project is to upgrade regularly using contemporary hardware decommissioned recently by large, national supercomputer installations. Because the RS/6000 SP system is a widely used and aggressively developed architecture, running such hardware is considerably more effective for supporting research in QTP than building a Beowulf cluster: The Xena strategy does not involve a one-time effort to build a system that quickly becomes obsolete, but focuses on frequent, periodic refreshes to stay within a constant technological distance of the leading-edge systems as they are deployed in national centers. In this strategy QTP is doing as an institute what U. Michigan and U. Texas are doing as institutions.

The Beowulf concept started to become well-known after NASA built a 16 node system of computers assembled from "off the shelf" sources, essentially PCs. However, the nodes ran the Linux operating system and were interconnected via standard Ethernet. The MPI message-passing programming model allowed all 16 nodes to work on a single problem. The cluster was named after the characters in the medieval poem telling the story of the hero Beowulf. Like the hero, the cheap cluster technology was fighting dragons: the dragon of “expensive supercomputers”. The software infrastructure for management of 16-node cluster was primitive compared to that in use on massively parallel supercomputers of the time (IBM SP2, Kendall Square KSR-2, Cray T3E). By comparison, the software infrastructure and system architecture developed in QTP since 1987 under the leadership of G. D. Purvis to manage the cluster of 50 Sun 3/50’s as a distributed system presenting a single system interface was more advanced than the Beowulf infrastructure in 1994. The only new element in the Beowulf cluster was use of the MPI library for parallel computations. Most Beowulf clusters in the world now are not used for large-scale parallel computations, but as a way to provide lots of scalar or small-scale parallel compute cycles to research groups. In comparison to the software infrastructure for high-performance computing developed for the IBM RS6000/SPs, the Beowulf infrastructure is still primitive, particularly in regard to the demands of algorithms typical of QTP’s research.

The Xena phase I configuration is well-suited for much of QTP’s research. However, the small amount of RAM (64 MByte) and disk space in each node are major barriers for other projects. The main reason is that even in parallel mode most QTP codes require significant local storage. Therefore QTP responded swiftly with a proposal when, in Sept. 2000, the Department of Defense High Performance Computing Modernization Program announced competitive availability of a major parallel supercomputer for award to DoD-sponsored labs and institutions. After extended study by the cognizant DoD office and
In addition to visualization of computed data, the lab will be used for training sessions and for classes in parallel programming, visualization, and simulation techniques. When not in use for visualization and imaging, the machines will run simulation calculations under a batch system.

The visualization lab also will house a 3D Quasi-Immersive Visualization (“virtual reality”) system funded by an NSF Instrumentation for Materials Research grant to Profs. Trickey, Stanton (Physics), Cheng, and Krause. This system consists of a Fakespace Inc., model R2 Immersadesk driven by an SGI Onyx 2000 with 4 CPUs/8GB of RAM and 45GB of disk. The Onyx 2000 was acquired with the help of a donation to Physics from Delta Airlines. The objective of the Quasi-Immersive Visualization effort is to learn how to probe 3D renderings of computed fields (quantum mechanical densities, trajectories, etc.) to detect internal relationships that otherwise are not apparent.

Security Enhancements for Research Flexibility

From its beginning, the Slater Lab has taken pains to work from a closely-reasoned system architecture to decide what to do when new technology comes along or new challenges arise. This Spring that architectural base allowed us to improve network security by using a new technology supported by the Solaris 7 operating system: logical interfaces. This technology allows us to attach mobile hosts and hosts for which the security is not completely up to standard to the QTP network by giving them a private IP address. Those addresses are blocked at the Physics Building router. Thus these classes of hosts can reach local QTP and Physics hosts, without the fear of being scanned from the Internet for known vulnerabilities. In a research environment such as QTP, the flexibility to attach such “non-supported” hosts to the network is increasingly important. By use of private IP, we avoid the security risks associated with putting Windows, Mac, or Linux hosts on the network. QTP now fully supports Solaris and AIX systems to the point of allowing them on the public Internet. All other systems are allowed with private IP only.

Enhanced Visualization of Scientific Data

The Xena project means that QTP members are able to compute the properties of bigger, more intricate systems with more sophisticated methods than before. Those scaleups generate their own challenge: finding the key patterns and new insights in unprecedented masses of data. Though great progress has been made in computational pattern recognition, it remains true that the human brain inspecting a suitably rendered image of a data field is the most potent pattern recognition system presently available. Therefore QTP members worked hard this year to bring a qualitatively new level of visualization capability and capacity.

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Funded by an IBM Shared University Research award to Prof. Hai-Ping Cheng and matching from the University of Florida (Dept. of Physics, College of Liberal Arts and Sciences, Office of Research and Graduate Programs) as well as QTP funds a new visualization and simulation lab opened in June 2001. The Department of Physics made available room NPB 1213. It houses six IBM RS/6000 44P-270 machines for simulation. Each machine has four (4) 375 MHz superscalar CPUs capable of 1.5 GFlops each, 3 GByte RAM, and 18 GByte disk, plus three smaller model 170 systems.
The 41st Annual Sanibel Symposium was held February 24 through March 2, 2001. Again the program attracted close to three hundred chemists, molecular and condensed matter physicists, molecular biologists, and other scientists; mostly theoreticians, but also experimentalists. These diverse of scientists share common interests in the development of theory and computational methods and their application to chemical and physical processes using large-scale computations. Participants from over thirty different nations made this meeting truly international in character. The Ponce de Leon Conference Center at the north gate of the historical city of St. Augustine, Florida, provided a comfortable setting for the symposium as it has for the past several years.

In addition to financial support from the University of Florida, the Symposium received support from the US Office of Naval Research, and the International Business Machine Corporation. As has been the case every year, the faculty, students and staff of QTP planned, organized, and ran the Symposium. The plenary lectures and poster sessions make it possible for almost all participants to present their work and to discuss with experts from a wide range of research areas. Breaks in the scheduled events and the various social functions make possible personal interactions between junior and senior scientists from around the world. Future collaborative research and employment opportunities derive from these contacts.

A distinguishing characteristic of the Sanibel Symposia is that they embrace many different scientific backgrounds, methodologies, and even conceptual structures. It is common to observe heated discussions between formal mathematicians and physical chemists, or between theoretical physicists and theoretical chemists. In particular, it is notable how in recent years biological and physical scientists interact and increasingly are beginning to learn from each others vocabulary. This catholic flavor of the Symposia distinguishes them among scientific conferences in these times of increasing specialization. In addition, the Symposia mix senior, well-established scientists, with graduate students and aspiring postdoctorals. The popular poster sessions, which by tradition open with a plenary session giving each scientist two minutes to advertise his/her poster, attracts presentation by young and old from undergraduates to Nobel Laureates.

IBM supported six competitive fellowships for promising young scientists attending the Sanibel symposia. The winners of the IBM-Löwdin fellowships were Dr. Pedro A. Rosa, University of South Carolina, Dr. Robert Ddanitz, University of Utah, and Dr. Valentín Karasui, Instituto Venezolano de Investigaciones Científicas. The winners of the IBM-Zerner fellowships were Mr. Mihály Kallay, Eötvös University, Ms. Daniela S. Mainardi, University of South Carolina, and Ms. Neepa T. Matra, Rutgers University. John Wiley & Sons supported two awards to young investigators participating in the symposia. The winners of the 2001 “Wiley Young Investigator Awards” were Dr. Deborah G. Evans, University of New Mexico, and Dr. David D. Scherrill, Georgia Institute of Technology. The awards and the fellowships, consisting of one thousand dollars, the symposium registration fee, and a plaque were presented at the banquet Wednesday evening of the symposium week.
The proceedings of the Symposia are published by the International Journal of Quantum Chemistry, (John Wiley and Sons) and edited by QTP faculty. These proceedings have a wide circulation and cover the science exhibited both in the plenary sessions and the poster presentations. This year’s proceedings contain over fifty-five papers.

Already the planning for the 42nd Sanibel Symposium is well under way and we expect to see participants from all over the world gather at the Ponce de Leon Conference Center for the week of February 23 through March 1, 2002.

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2001 Pan-American Workshop on Molecular and Materials Sciences: Theoretical and Computational Aspects

February 21-23, 2001
Gainesville, Florida

David A. Micha and Samuel B. Trickey
Organizers

The purpose of this workshop was to promote scientific contacts among scientists in the US, Latin America, Canada, and the Caribbean aimed at developing theoretical and computational methods applicable to problems of common interest in the molecular and materials sciences, and at encouraging long term collaborations with those scientists as they return to their countries. The workshop had 47 participants from eight countries. The subjects covered many-electron theory of molecular properties, their interaction with electromagnetic fields, and intermolecular interactions, including also solvation effects, many-electron theory of solids, proteins, and clusters, and in particular density functional theories, quantum theories of molecular dynamics and spectra, and time-dependent many-electron treatments of electronic dynamics, as well as their computational aspects.

Participants had the opportunity to proceed to the 2001 Sanibel Symposium, organized also by the University of Florida immediately after the workshop in St. Augustine, Florida, to interact with scientists from the US and many other countries.

This 2001 workshop was the fifth in a series started at the University of Florida. The previous one was organized in 1999, at the Centro de Ciencias Físicas in Cuernavaca, Mexico, which has also been selected as the site of the next workshop, planned for February of 2003. Workshop activities have been recorded in proceedings with abstracts of presentations.
We Can Do That!

An International Symposium in Honor of Michael Zerner

November, 16-18, 2000
Gainesville, Florida

John R. Sabin, with the faculty and staff of QTP

Our friend and colleague Mike Zerner died on February 2, 2000, after a long and difficult battle with cancer. We, his friends and colleagues from all over the world, and from many fields in theoretical chemistry and physics, held a symposium in his memory in Gainesville on the weekend of 16 - 18 November, 2000. We gathered to discuss science and to remember Mike.

The topics covered in this Symposium were those with which he was most concerned. To wit:

- Semi-empirical methods
- Solvation & Environmental Effects
- Biochemical problems
- *ab initio* theory

Invitational Symposium on Novel Computational Approaches to Low-Energy Atom-Atom and Atom-Ion Scattering

February, 2001
Gainesville, Florida

John R. Sabin and Frank Harris
Organizers

At the University of Florida and other institutions, active research programs are studying novel theoretical methods for treating low-energy inelastic atom-atom and/or atom-ion scattering. This work is computationally intensive and valuable in that it describes processes that are important in both terrestrial and astrophysical chemical applications, as well as those occurring in the modelling of fusion plasmas and slow collisions involving antiparticles. This work has now reached a point where an interchange of insights and experience among the researchers would be highly beneficial, and this Symposium was designed to help meet this need.

Topics discussed included Electron Nuclear Dynamics (END)-Theory (Yngve Õhrn, University of Florida); ENDYNE--The Implementation of END (Erik Deumens, University of...
Florida; Collision Cross Sections Calculated with END (John R. Sabin, University of Florida); First Principles Dynamics of Many-Electron Atom-Atom Collisions (David A. Micha, University of Florida); The Hidden Crossings Approach for Slow Atomic Collisions (Pedrag Krstic, Oak Ridge National Laboratory); Solutions of the Time-Dependent Schrödinger Equation (David R. Schultz, Oak Ridge National Laboratory); R-Matrix Theory and Calculations (H. Harvey Michels, University of Connecticut); Taking Quantum Chemistry into the Complex Plane of Internuclear Distance (Gary D. Bent, University of Connecticut), and a round table discussion on Complex Scaling and Hidden Crossings Theory.

**Workshop on Atomic, Molecular, and Optical Physics at Surfaces**

June 14-16, 2001  
Cambridge, Massachusetts  
David A. Micha, Uwe Thumm, and John Tully  
Organizers

This workshop was organized as part of a series at the Institute for Theoretical Atomic and Molecular Physics, a National Science Foundation Center located at the Harvard-Smithsonian Center for Astrophysics. It covered molecular dynamics, adsorption, dissociation, and desorption, scattering of atoms, molecules, ions and excited atoms, cold atom collisions, and electron of emission and transfer, with presentations by 22 participants and attendance of 30 researchers.

Abstracts, viewgraphs, and audio of the presentations can be found at the web site of the ITAMP.

**Sixteenth International Conference on Application of Accelerators in Research and Industry**

October 13, 2000  
University of North Texas  
John R. Sabin and Samuel B. Trickey  
Session Organizers

Two sessions of invited talks on “Charged Particle Energy Depositions in Novel Material and Molecular Systems” at the Sixteenth International Conference on Application of Accelerators in Research and Industry were organized by John R. Sabin and Samuel B. Trickey.
2001 Lectures

Robert K. Nesbet
IBM Almaden Research Laboratory

One of the major figures in the early development of Quantum Mechanics, especially for many-electron systems, Professor Slater played a major role in the early years of QTP (see QTP's History in this report or on the Web). One of his many contributions was to give comprehensive reports on state-of-the-art research in the format of three or four closely spaced lectures.

To enrich the research environment of QTP and honor that tradition, we began this year what will be an annual event, the John C. Slater Lectures. The first lecturer was Robert K. Nesbet, IBM Almaden Research Laboratory. Both Dr. Nesbet's background and lecture series topic were remarkably appropriate to the Slater legacy. Early in his career, Dr. Nesbet did a postdoctoral stint with Prof. Slater. His lectures concerned subtle questions in the area of Density Functional Theory. Much of the latter part of Slater's career was focused on an approximate version Density Functional Theory.

The Lectures were entitled “Local and Nonlocal Potentials in Density Functional Theory.” The daily titles were:

Feb. 15, 2001
Thesis: Are Density Functional Derivatives Really Local Functions?

Feb. 16, 2001
Antithesis: Orbital Functional Derivatives Define Linear Operators

Feb. 20, 2001
Synthesis: All Exact Theories are the Same
FACULTY

Rodney J. Bartlett
Graduate Research Professor of Chemistry and Physics

Hai-Ping Cheng
Associate Professor of Physics

Erik Deumens
Associate Scientist of Chemistry and Physics
QTP Computing Director

Frank E. Harris
Resident Adjunct Professor of Chemistry

Jeffrey L. Krause
Associate Professor of Chemistry

David A. Micha
Professor of Chemistry and Physics

Hendrik J. Monkhorst
Professor of Physics and Chemistry

N. Yngve Öhrn
Professor of Chemistry and Physics

Adrian E. Roitberg
Assistant Scientist of Chemistry

John R. Sabin
Professor of Physics and Chemistry
D.I.R.T., CLAS

Samuel B. Trickey
Professor of Physics and Chemistry
Director, QTP

ADJUNCT FACULTY

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University of Waterloo
Canada

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Youngstown State University
Ohio

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Århus University
Denmark

William H. Miller
University of California Berkeley

Jens Oddershede
Odense University
Denmark

Neil S. Ostdlund
Hypercube
Florida

Josef Paldus
University of Waterloo
Canada

VISITING ASSISTANTS

So Hirata
Chemistry (Bartlett)

Ajith S. Perera
Chemistry (Bartlett)

Piotr Rozyczko
Chemistry (Bartlett)
POSTDOCTORAL ASSOCIATES

Araf Al Derzi
Chemistry (Bartlett)

Marshall Cory
Chemistry (Bartlett)

Pilar de Lara
Chemistry (Krause)

Stefan Fau
Chemistry (Bartlett)

Norbert Flocke
Chemistry (Bartlett/Trickey)

Ireneusz Grabowski
Chemistry (Bartlett)

Thomas Herz
Chemistry (Sabin)

Andrew Kolchin
Physics (Cheng)

Svetlana Malinovskaya
Chemistry (Sabin)

Vladimir Malinovsky
Chemistry (Krause)

Keith Runge
Physics (Bartlett)

Krassimir Stavrev
Physics (Sabin)

Qi-Heng Tang
Physics (Cheng)

Remigio Trujillo
Physics (Sabin)

Sergio Urahata
Chemistry (Sabin)

Jianjun Xu
Physics (Cheng)

GRADUATE STUDENTS

Ariana Beste
Chemistry (Bartlett)

Anatol Blass
Chemistry (Öhrn)

Mauricio Coutinho-Neto
Chemistry (Öhrn)

Maohua Du
Physics (Cheng)

Shannon Greene
Chemistry (Krause)

Thomas Henderson
Chemistry (Bartlett)

Ben Killian
Chemistry (Öhrn)

Corneliu Manescu
Physics (Krause)

David Masiello
Chemistry (Öhrn)

Wilfredo Ortiz
Chemistry (Krause)

Ted O’Brien
Chemistry (Zerner/Sabin)

Alexander Pacheco
Chemistry (Micha)

Andres Reyes
Chemistry (Micha)

Eve (Tina) Rivera
Chemistry (Roitberg)

Alberto Santana
Chemistry (Micha)

Igor Schweigert
Chemistry (Bartlett)
Graduate Students

Kevin Shuford
Chemistry (Krause)

Guangyu Sun
Physics (Tricke)

DeCarlos Taylor
Chemistry (Zerner/Bartlett)

Brian Thorndike
Physics (Micha)

Motoi Tobita
Chemistry (Bartlett)

LinLin Wang
Physics (Cheng)

Ken Wilson
Chemistry (Bartlett)

Anthony Yau
Chemistry (Bartlett)

Chun Zhang
Physics (Cheng)

Wuming Zhu
Physics (Tricke)

Undergraduate Students

Ryan Chancey
Chemistry (Bartlett)

Gareth Forde
Chemistry (Harris)

Ashleigh Hermansen
Chemistry (Krause)

Anthony Hernandez
Chemistry (Micha)

Chris McKenny
Chemistry (Harris)

Lane Newsom
Chemistry (Sabin)

Ramiro Rojas
Chemistry (Harris)

Kevin Tidgewell
Chemistry (Bartlett)

Sebastien Vallaume
Chemistry (Micha)

Meng Wei
Physics (Harris)

Staff

Janice Barner
Program Assistant (Bartlett)

Coralu Clements
Senior Word Processing Operator

Long Duong
Program Assistant (Bartlett)

Erin Graul
Fiscal Assistant

Cindy LePrell
Senior Secretary

Judy Parker
Office Manager

Arlene Rorriguez
Senior Secretary

Student Office Assistants

Jessica Bentele

Viveka Lazor

Megan Roessner

Degree Granted

Ted O’Brien, Ph.D. under the direction of M.C. Zerner and John R. Sabin, October 2000.
Bartlett

Ab Initio Density Functional Theory, 4th Canadian Computational Chemistry Conference, Bishop’s University, Lennoxville, Québec, Canada, July 2000.


NMR Coupling Constants Across Hydrogen-Bonds: The Role of Predictive Theory, University of Tennessee, Knoxville, Tennessee, August 2000.


Prospects for Polynitrogen HEDMS, DARPA Polynitrogen HEDM Program, Salt Lake City, Utah, October 2000.


NMR Coupling Constants Across Hydrogen-Bonds: The Role of Predictive Theory, Purdue University, West Lafayette, Indiana, April 2001.


Cheng


Quantum Simulation of Water Cluster: Proton and Double Hydrogen Transfer, Department of Physics, Göteborg University and Chalmers University, Göteborg, Sweden, March 2001.


Using the QTP Computing Laboratory, QTP, University of Florida, September 2000.

Programing with Open MP, Brigham Young University, March 2001.

Introduction to Parallel Programming. Florida State University, Florida, April 2001.

Scientific Work and Mounaineering with Per-Olov Löwdin, Uppsala University (Sweden), October 2000.


Leaky Aquifer Functions and Their Role in Extended-System Hartree-Fock Calculations, University of Leuven (Belgium), January 2001.


Toward Exact Hartree-Fock Calculations in Extended Systems, Physics Division, Oak Ridge National Laboratory, June 2001.


Quantum Control of Wave Packet Dynamics, Georgia Institute of Technology, Atlanta, Georgia, May 2001.


First Principles Collision Dynamics of Electronic Energy and Charge Transfer; Institute for Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, December 2000.


Electron Nuclear Dynamics, Recent Progress, at University of Copenhagen, Denmark, August 2000.


Electron Nuclear Dynamics, National Chemistry Laboratory, Pune, December 2000.


Nonadiabatic Treatment of Ion-atom, and Ion-molecule Collisions, Theoretical Physics Inst. of Mathematical Sciences, Madras (Chennai), December 2000.

Electron Nuclear Dynamics, Jawaharlal Nerhu University, Delhi, lecture Tour of Indian Institutions, December 2000.


An MD/QM Investigation of the Chorismate Mutase Catalyzed Claisen rearrangement, George Mason University, Fairfax, VA, November, 2000.


POL, UF, & QTP, Löwdin Memorial Symposium, Uppsala, Sweden, October 2000


Shape Dependent Molecular Properties: Energy Deposition, 16th International Conference on the Application of Accelerators in Research and Industry, Denton, Texas, November 2000.


Shape Dependent Molecular Properties: Energy Deposition, Danish Chemical Society Annual Meeting, Odense, Denmark, June 2001.


N. Rostoker, M.W. Binderbauer and H.J. Monkkorston, “Colliding Beam Fusion Reactors with Pulsed  


R. Cabrera-Trujillo, E. Deumens, Y. Öhrn, J.R. Sabin, “Impact Parameter Dependence of Electronic and  

R. Cabrera-Trujillo, J.R. Sabin, Y. Öhrn and E. Deumens, “Charge Exchange and Threshold Effect in the  

R. Cabrera-Trujillo, Y. Öhrn, E. Deumens, J.R. Sabin, “Stopping Cross Section in the Low- to Interme-

R. Cabrera-Trujillo, J.R. Sabin, E. Deumens, Y. Öhrn, “Stopping Cross Section and Charge Exchahge  


A.E. Roitberg, Sharon Worthington, Marcia J. Holden, Martin P. Mayhew, and Morris Krause, “The  
Electronic Spectrum of thePrephenate Di-Anion. an Experimental and Theoretical (MD/QM) Com-

V. Mujica, A.E. Roitberg, and M.A. Ratner, “Molecular Wire Conductance: Electrostatic Potential Spat-


S.E. Worthington, A.E. Roitberg, and M. Krauss, “A Theoretical Study of the Chorismate Mutase Cata-


BOOKS

*Advances in Quantum Chemistry*
John R. Sabin and Erkki Brändas, Editors

*Finite Systems and Multiparticle Dynamics*
Book Series by Plenum Press
David Micha, Senior Co-Editor

*Proceedings of the 2001 Sanibel Symposium*
*International Journal of Quantum Chemistry*
Yngve Öhrn, Editor; John R. Sabin, Associate Editor

JOURNALS

*International Journal of Quantum Chemistry*
Yngve Öhrn, Editor; John R. Sabin, Associate Editor

*Computer Physics Communications*
Samuel B. Trickey, Specialist Editor (*Condensed Matter Physics*)
Jan Broeckhove  
R. U. C. A.  
Antwerp, Belgium  

Jan Linderberg  
Aarhus University  
Aarhus, Denmark  

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Youngstown State University  
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University of Namur  
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Uppsala, Sweden  

Jose A. Recamier  
Universidad Nacional Autonoma de Mexico  
Cuernavaca, Mexico  

Stanislaw Kucharski  
Silesian University  
Katowice, Poland  

Isaiah Shavitt  
Ohio State University  
Columbus, Ohio  

Roland Lindh  
University of Lund  
Lund, Sweden  

Brian L. Weiner  
Pennsylvania State University  
DuBois, Pennsylvania
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<td><em>Pseudo-Jan-Teller Interactions and Conical Intersections in Coupled-Cluster and Many-Body Perturbation Theories</em></td>
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<td>Dr. Samuel Trickey, Director of QTP</td>
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In the late 1950’s
then Graduate Dean Linton E. Grinter, Chemistry Chair Harry H. Sisler, and Physics Chair Stanley S. Ballard, all of the University of Florida, had the idea to create a strong presence in the emerging field of Theoretical Chemical Physics and Quantum Chemistry. To lead that charge they selected a dynamic scientist with exceptional energy and unique abilities to realize his dream of creating a truly international research and teaching program. That choice defined the development of the Quantum Theory Project for many years.

The arrival of Per-Olov Löwdin (as Graduate Research Professor of Chemistry and Physics) at the University of Florida in 1960, immediately followed by the appointments of a number of junior faculty (visiting and permanent), marks the inception of the Quantum Theory Project (QTP), an institute for research and graduate education in the areas of Theoretical Chemical Physics and Physical Chemistry. The name itself is worth a historical aside. Long since shortened, the original title was “Quantum Theory Project for Research in Atomic, Molecular and Solid State Theory”.

From the beginning QTP was not a separate unit but a joint program of two basic academic disciplines, Chemistry and Physics. Thus, in 1960 the Department of Physics hired John S. Faulkner and Richard F. Wood as Assistant Professors and the Department of Chemistry similarly hired Darwin W. Smith. Those three young scientists, together with then Associate Professor Charles E. Reid (already on the Chemistry faculty) joined Löwdin to form the initial permanent faculty of the QTP. Both Faulkner and Wood spent some time that first year at the Quantum Chemistry Group of Uppsala University in Sweden, Löwdin’s home institution, and several young scientists from Uppsala spent one to two years at UF. In this way an exchange of scientists was started between the University of Florida and Uppsala University in QTP’s specialties. That particular exchange has continued while the tradition of exchanges has been expanded to include other institutions.

The first contingent from Uppsala to hold positions of visiting Assistant Research Professors in the QTP consisted of Klaus Appel, Jean-Louis Calais, and Jan Linderberg (1960-61), Jan Nordling (1961-62), and Yngve Öhrn (1961-63). Other visiting scientists for extended periods during these early years included Werner A. Bingel (Germany), Joseph O. Hirschfelder (Wisconsin), G. Ludwig Hofacker (Germany), Egil A. Hylleraas
(Norway), Harold V. McIntosh (RIAS, Maryland), Kimio Ohno (Japan), and Ruben Pauncz (Israel).

It is interesting to note where some of these pioneers, who came together at UF during the formative years of the QTP, later found more permanent employment. Appel became the Director of the University Computing Center at Uppsala. Calais was Associate Professor of Quantum Chemistry at Uppsala University. Both are now deceased. Linderberg holds the chair of Theoretical Chemistry at Aarhus University in Denmark. Nordling is now Lecturer at Sundsvall University College in Sweden after concluding a successful career in the private computer industry. Öhrn is Professor of Chemistry and Physics at UF since 1966. Bingel held the chair of Theoretical Chemistry at the University of Gottingen in Germany until his retirement a few years ago. Hirschfelder was already at the time one of the scientific pioneers in the field and held the position of Professor at the University of Wisconsin. He died in 1990. Hylleraas, one of the originators of the field of computational molecular physics, held the chair of Theoretical Physics at Oslo University in Norway. He passed away in 1967. Hofacker retired (1998) from the chair of Theoretical Chemistry at the Technische Universität at Munich in Germany. McIntosh became professor at Universidad de Puebla, Mexico. Ohno, now retired, held the chair of Theoretical Chemistry at Hokkaido University, Japan. Pauncz was Professor of Chemistry at Haifa University in Israel until his retirement a few years ago. Faulkner and Wood left QTP in 1964 to take group leader positions at the Oak Ridge National Laboratories. Faulkner joined the physics faculty at Florida Atlantic University. Smith left UF in 1967 for the chemistry faculty at the University of Georgia. Those early years established the tradition, which is still very much alive and valuable today, of having a number of active scientists from all over the world as visitors in QTP. This practice created a uniquely open and fertile environment for the exchange of ideas, as well as a truly international network of colleagues and friends.

From the beginning, QTP faculty understood the value of communicating the latest in research findings to graduate students and other young as well as senior scientists eager to join the growing community of quantum chemists and chemical physicists. At that time there were almost no courses and few textbooks on the subject. To fill that gap QTP began annual Winter Institutes (WI) on Quantum Chemistry, Solid State Physics, and Quantum Biology in 1961. These extremely intense courses, lasting for six weeks or longer, had their first part on the UF campus. Many senior scientists from around the world visited UF for shorter periods during the WI. Looking through a list of those names is almost like reading a worldwide Who’s Who in those fields of study.

The Winter Institutes were partitioned into a Preparatory Part, and one or two Advanced Parts. The last two weeks on the WI were held on Sanibel Island, just off Ft. Myers, Florida in the Gulf of Mexico. From the second year the site was the Casa Ybel Resort, which provided a unique nature setting, albeit primitive facilities. (Casa Ybel was a quaint collection of modern beach cottages,
1920’s beach cottages, motel units, and partitioned old houses most of which had seen better days.) The Sanibel part concluded with a one week Symposium, which attracted active scientists from around the world for a conference program that can be characterized as intense and exhausting. Typically the scientific sessions ended at midnight and started at eight thirty in the morning. A total of about 250 participants came each year to the WI and the Sanibel Symposium.

It is fair to say that these activities had a significant impact on chemical physics and physical chemistry in a variety of ways. At most institutions throughout the world a theorist in these fields, such as a quantum chemist, was, and often still is, the only person with that specialty on the faculty. To meet a colleague with similar interests and scientific expertise often would require significant travel. Given that scenario, it is understandable that the yearly WI and Sanibel Symposium were embraced with sustained enthusiasm among these scientists. Here was a series of events, concentrated in time and space which made it possible for senior scientists, postdoctoral associates, and graduate students to meet most of the world’s experts in the specialty, to learn about the latest developments, and to disseminate their own work among this group for the cost of one trip to Florida.

In Fall 1964 a major influence on QTP’s evolution arrived in the person of John C. Slater, appointed as Graduate Research Professor of Physics and Chemistry. Slater had been Professor and Chair of the Department of Physics at MIT and had established the Solid-State and Molecular Theory Group (SSMTG) there. Löwdin had visited MIT in the 1950’s and established strong contacts with this internationally known group. The arrival of Slater meant a considerable strengthening of QTP in the area of condensed matter theory. James B. Conklin Jr., also from MIT, was appointed Assistant Professor of Physics the same year. In 1966 Yngve Öhm joined the QTP faculty as Associate Professor of Chemistry and Physics, and in the same year Donald E. Ellis took the position as Assistant Professor of Physics. Ellis left in 1968 to join the Physics Department at Northwestern University where he is today. Timothy M. Wilson, a QTP graduate, held the position of Assistant Professor of Physics 1968-69, after which he joined the Physics faculty at Oklahoma State University. In 1968 Samuel B. Trickey (current Director of QTP) came to the Florida Physics Department and joined QTP in 1969. Another current member of QTP, David A. Micha, joined the Chemistry faculty as an Associate Professor that Fall. He had spent some time as an Assistant Research Physicist in Keith Brueckner’s group at the University of California, La Jolla after earning his graduate degrees at Bariloche, Argentina, and Uppsala, Sweden, and doing postdoctoral work at the University of Wisconsin, Madison. John R. Sabin, also

“The Sanibel Symposium attracts about 350 scientists every year from over thirty different nations”
a current member of QTP, joined the group from the University of Missouri in 1970, first as a temporary replacement for Yngve Öhrn, who spent the year at Aarhus University in Denmark, and later as a permanent faculty member of the Department of Physics. In 1970, a QTP graduate, John W. Connolly, returned to take the position of Associate Professor of Physics. After graduation he had been a scientist with United Technologies.

In 1976 Conklin left the group to become the first Director of CIRCA, the instructional computing group at UF. Even before that time Conklin and Slater had both played roles in the early leadership of the UF Computing Center. In 1976 Slater died.

Shortly thereafter Connolly left to join the National Science Foundation, where he held several positions of importance, perhaps most notably as the first program director of the NSF Supercomputer initiative. Today he heads a scientific computing center at the University of Kentucky. Trickey left in 1977 to become Chair of the Department of Physics at Texas Tech University. He returned to QTP in 1979. The same year another current QTP member, Hendrik J. Monkhorst, joined UF as Associate Professor of Physics. Educated in the Netherlands, he had spent several years in the University of Utah Physics Department working in close collaboration with Frank E. Harris, a regular lecturer at the Winter Institutes.

A major expansion of the QTP program took place in 1982 with the appointments of Rodney J. Bartlett, a QTP graduate, and Michael C. Zerner as Professors of Chemistry. Zerner died in February 2000.

In 1980 QTP made its first small foray into operating its own computers, a move delayed by various state rules. In 1982, the QTP Computing Facility was created, the position of Computer Manager was established, and George D. Purvis III, also a QTP graduate, was hired as an Associate in Chemistry for that post. Bartlett and Purvis had held scientific staff positions at Battelle Laboratories in Columbus, Ohio, and Zerner had been Professor of Chemistry at Guelph University in Canada. Bartlett was promoted to Graduate Research Professor in 1987. In 1988 Erik Deumens, from Antwerp University in Belgium, succeeded Purvis, who moved to CAChe Scientific, Beaverton, Oregon as Vice President for Research and Development. The latest additions to the QTP permanent faculty have taken place in the last few years. Hai-Ping Cheng, with a Ph.D. degree from Donald Ellis at Northwestern, and Jeffrey Krause, with a Ph.D. degree from Stephen Berry at the University of Chicago, joined Physics (1994) and Chemistry (1994) respectively. Both are now Associate Professors. In January 2001, Adrian E. Roitberg joined the Institute as an Assistant Scientist (chemistry) specializing on predictive simulations of biomolecules and on software support for the JCS computing laboratory.

When QTP was founded, the University of Florida had no formal structure for such an interdisciplinary institute. For almost twenty-seven years QTP was an informal association of a number of Chemistry and Physics faculty members and their research groups. By 1986, in response to a general feeling among its faculty that QTP had outgrown the informal form, the possibilities for a more formal structure were explored. In 1987 the result was a reorganization as the “Institute for Theory and Computation in Molecular and Materials Sciences.” However, convenience and familiarity prevail and the Institute still is generally known as QTP. Under the reorganization QTP is, in the jargon of the state of Florida, a type-II institute, with its own bylaws and a modest budget. It continues to be an integral part of the programs of the Chemistry and Physics Departments of UF. The first elected Director of this Institute was Yngve Öhrn, who stepped down at the end of 1998 and was succeeded by Samuel B. Trickey who is serving in that capacity. Trickey earlier had served as the first elected Computer Director of the Institute, an important responsibility now held by Erik Deumens.

The Winter Institutes have become less frequent. The latest one (held in 1988) had participants primarily from the Latin American Countries. The growing interest for meaningful collaboration with QTP from scientists in Central and South America has led to the organization, by David Micha, of two three-day research meetings on the UF campus preceding the Sanibel Symposium. This Latin American Workshop attracts between thirty and forty scientists each year from universities in Latin America and the Caribbean Basin.

In contrast, the Sanibel Symposia have been held in an unbroken string of annual gatherings. In 1978 the site of the meeting was changed from Sanibel Island, as a consequence of the sale of the Casa Ybel property for real estate development. The new location at Palm Coast (on the East Coast of Florida), was quite a bit closer to the UF campus, and the Sheraton Hotel there served as an excellent symposium site until 1985. That year the meeting was moved a couple of miles further North along highway A1A to the Whitney Marine Biological Laboratories of UF at Marineland. In 1989 the Sanibel Symposium (the name of the original site has been permanently attached to this meeting) had outgrown the facilities at Marineland and a new site was found just outside the North gate of St. Augustine, Florida, the oldest European settlement in the United States. Ponce de Leon Conference Center has housed the symposia since then, except for 1994, when the meeting went to the Marriott at Sawgrass, about seventeen miles north of St. Augustine on the Atlantic coast. The Sanibel symposium at-

“"The scientific achievements of the scientists associated with QTP are numerous and cover many sub-fields"
tracts about 350 scientists every year from over thirty different nations. It has become an integral part of the activities of QTP. In 2000 the 40th symposium took place.

A one week course in Applied Molecular Orbital Theory under the directorship of Rod Bartlett, primarily intended for chemists in industry was part of the QTP agenda for several years. Typical attendance was twenty to thirty and the program involved several QTP faculty, postdoctoral associates, and graduate students. Bartlett has also conducted several ACES II workshops.

For the past two years, QTP faculty in the KDI project have conducted a summer undergraduate research program. Several chemistry and physics REV students have done their research in QTP as well.

The Institute faculty serve on the editorial boards of many of the primary journals in chemical physics and theoretical chemistry. The editorial offices of Advances in Quantum Chemistry and the International Journal of Quantum Chemistry are housed in QTP. Faculty members are active also in national organizations. Bartlett has served as Chair elect and Chair of the Theoretical Subdivision of the Physical Chemistry Division of the American Chemical Society. Micha served as Vice Chairman and Chairman of the Few Body Physics Topical Group of the American Physical Society. Trickey has served as chair of SUPER!, a national organization of (mainly academic) supercomputer users associated with IBM.

Some QTP faculty have served the University in administrative roles as well. Öhrn was Chairman of Chemistry (1977-1983), as was Zerner (1988-1994). Trickey was Director for Information Technologies for the College (1986-1990) and Executive Director for the Office of Information Technologies and Services at UF during 1991-1996. David Micha was the cofounder of the Center for Chemical Physics and served as its first elected Director (1982-1991). Sabin has been the College Information Technology Director since 1998.

The QTP faculty have had the good fortune to work with a dedicated secretarial and clerical staff. Eleanor J. Fox, Philamena V. Pearl, Jacquelyn M. Davis, Evelyn J. Smith and Phyllis Durre carried much of the secretarial and administrative responsibilities during the sixties. Drucilla Bouffard, Josephine Larrauri, Charlotte Rustin, Laura Steward, Charlene Catlett, Daryl Moore, Brenda Foye, Joyce Christianson, Susan Lyon, Robyne Stewart and Susan Janis served with distinction during the seventies. Joanne Bratcher, Cynthia Karle, Arline Succow, Vivian Goeller, Sylvia Whitten, Barbara Wubbels, Robin Bastanzi, Jody-Kate Fischer, Clara Reed, and Susan Linsley carried us through the eighties into the nineties. Leanne Golemo, Heather Lawhorn, Sharon Stellato, Kathy Fuller, Karen Yanke, Sandy Weakland, Janice Barner, Grace Kiltie, and Cynthia LePrell were staff for several years in the nineties. The current staff of Judy Parker, Coralu Clements, Arlene Rodriguez and Long Duong are carrying

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on the QTP tradition of hard work and dedication to the QTP mission. 
Associated with the QTP are a number of special individuals and frequent visitors, who have been given the distinction of adjunct QTP faculty. These include Jiří Cizek and Joseph Paldus of the University of Waterloo, Canada, William H. Miller, Professor of Chemistry at the University of California, Berkeley, Jens Oddershede, Professor of Chemistry, former Dean of Science and now Rector at University of Southern Denmark (Odense), Jan Linderberg, Professor of Chemistry at Aarhus University, Denmark. The newest, Janet Del Bene of Youngstown University, Pennsylvania. An important association was formed with Neil Ostlund, CEO of Hypercube in 1996, who opened a branch of his company in Gainesville and joined QTP as an adjunct faculty. In 1999 Frank E. Harris was voted a Resident Adjunct Faculty Member.

The scientific achievements of the scientists associated with QTP are numerous and cover many subfields. The early work of Löwdin introduced new theoretical techniques in the study of molecular electronic structure. Particularly his work on electron correlation has been of great importance. His introduction of the concepts of natural orbitals, bracketing functions, and lower bounds into the study of molecular systems are widely recognized. His comprehensive treatment of perturbation methods and mathematical studies of orthogonalization procedures and linear dependencies are central to applied quantum chemistry. His study of proton tunneling among base pairs with its implications for the stability of the genetic code brought quantum chemistry into the realm of biology. Slater developed the so called X form of approximate density functions theory, and with his students applied these ideas to a wide range of molecular and condensed matter problems. This work was is the precursor to the striking developments in density functional theory, primarily in condensed matter theory, but recently (and with sudden popularity) in chemistry as well. Some of the most detailed and comprehensive band theory calculations and associated computer codes were developed at QTP by Slater’s group. Slater wrote several of his classical monographs during his QTP tenure. Öhrn and Deumens developed and implemented the electron nuclear dynamics (END) theory, which is a time-dependent nonadiabatic approach to molecular processes. Micha developed and implemented few-body and many-body scattering methods and time-dependent many-electron methods for quantum molecular dynamics. Trickey developed and implemented rigorous ab initio treatment of thin films. Sabin pioneered novel methodology in the study of stopping of swift particles by various materials. Monkhorst adapted the coupled-cluster theory to the study of many-electron systems including the use of multireference cases, linear response properties, and nonadiabatic effects. Bartlett pioneered the development application of MBPT and coupled-cluster theory to molecules, including the development of the ACES II program system which offers general molecular applications for energies, gradients, excited states, and spectra. According to the Institute for Science Information (ISI) Bartlett is the 25th most cited chemist in the world (1981-97). Zerner developed and implemented the
widely used semi-empirical method known as ZINDO for the study of spectra and properties of truly big molecules including molecules with heavy elements. The capabilities of the ZINDO code include solvent effects and geometry optimization routines.

The research interests of the current QTP faculty include the study of elementary chemical reactions, spectroscopy and dynamics of molecules at solid interfaces (Micha, Öhrn, Deumens), the properties of thin films and surfaces, the effect of ionizing radiation on materials (Sabin, Trickey), density functional theory (Bartlett, Trickey), accurate calculation of molecular properties, determination of conformations of new molecular species, prediction of heats of formation (Bartlett), development of new methodology for theoretical studies of molecular electronic structure (Bartlett, Monkhorst), nonlinear optics (Bartlett), solvent effects (Micha, Zerner), multiscale simulation of complex biological phenomena (Roitberg) (Bartlett, Cheng, Harris, Trickey), nanostructures of materials, molecular dynamics, collisions of argon clusters with metal surfaces (Cheng), applications of new computer architectures to problems in chemistry (Deumens), laser control of chemical processes (Krause), time-dependent methods for properties and dynamics of molecular systems (Cheng, Deumens, Micha, Öhrn, Krause), novel methods for controlled fusion reactions (Monkhorst).

The impact of this research can be measured in various ways and the steady flow of visitors through QTP is an indication of the broad interest that exists in the research carried out. Also the numerous invitations that the institute faculty receives to speak at various national and international meetings and institutions is clear proof of the high regard in which the QTP research activities are held.