

QTP History

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".



*Per-Olov Löwdin
Sanibel Island, FL
early 1960's*



Uppsala 1982

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.



Jean Louis Calais

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).



*Jan Linderberg
early 1960's*

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.



Ruben Pauncz

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.



Casa Ybel, Sanibel Island, early 1960's

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.



John Slater

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 Öhrn 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



Sam Trickey



Rod Bartlett

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.



Mike Zerner



David Micha

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 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.



Jack Sabin



Erik Deumens

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.



Hai-Ping Cheng

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.



Henk Monkhorst

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.



Frank Harris



Jeff Krause

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.



Adrian Roitberg

In 2000, QTP suffered three losses. Zerner died February 2nd. Reid had retired in 1986 and while Professor Emeritus completed a revision of his book on thermodynamics. He died September 7, 2000. In 1992 Löwdin retired and became Professor

Emeritus. Until recently he maintained an active program with a steady flow of manuscripts. He died October 6, 2000.

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 attracts about 350 scientists every year from over thirty different nations. It has become an integral part of the activities of QTP. In 2002, the 42nd 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 REU 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



Session Break - Sanibel 2003

been the College Information Technology Director since 1998. The QTP faculty has 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 Wubbel, 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, Long Duong, Jason Hisey, Tom Connelly and Cynthia LePrelle were staff for several years through the nineties and beyond. The current staff of Judy Parker, Coral Clements, Arlene Rodriguez and Adam Web are carrying 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 Jiri 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



Janet Del Bene

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. scientific



Frank Harris

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



This unique triple crowned Sabal Palm, photographed at Kanapaha Gardens, Gainesville, Florida, is very much like the psi used as a symbol of QTP

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 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.

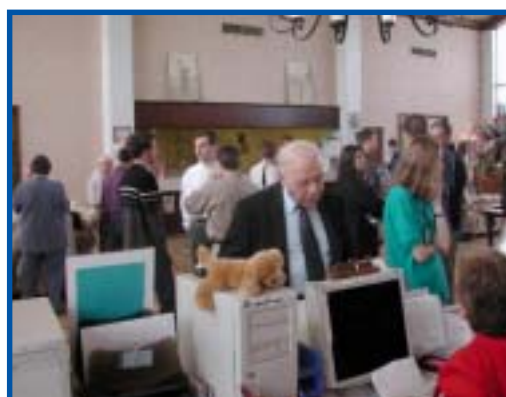
The research interests of the current QTP faculty include the study of elementary chemical reactions, spectroscopy and dynamics of molecules at solid interfaces (Micha, Öhrn, Deumens), the properties of thin films and surfaces, the effect of ionizing radiation on materials (Sabin, Trickey), density functional 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), nano-structures 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).

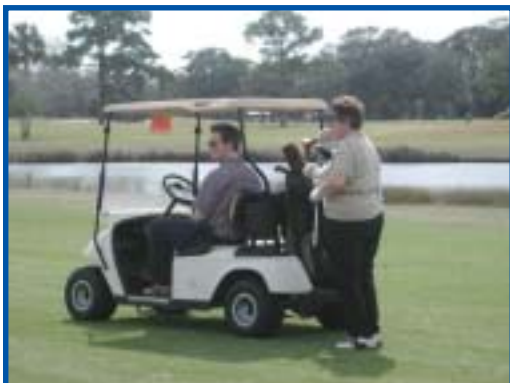
The impact of this research can be measured in various ways and the steady flow of visitors through QTP is an indication of the broad interest that exists in the research carried out. Also the numerous invitations that the institute faculty receives to speak at various national and international meetings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



Henk Monkhorst, Sam Trickey, and Stefan Fau with Afaf Al Derzi during her farewell party.



Jerome Karle registering at the 2003 Sanibel Symposium



The World's Greatest Quantum Golfer tournament, sponsored by Hypercube, is held during Sanibel; here, Janet Del Bene is ready to try her hand.



A QTP family Thanksgiving. Monika Musial, Tom Henderson, Remigio Trujillo (hidden), Luz Maria Diaz-Rivera, Charley VanMiddlesworth, Judy Parker, Ajith Perera, Alex Pacheco, Deepa Savant .



Hot and tired after unloading two semi-trailers full of computer equipment which, after Erik Deumens' magic, turned into Xena II. Standing: Remigio Trujillo, Kevin Shuford, Ken Wilson, Carlos Taylor, Adrian Roitberg, Sebastien Villaume. Sitting: Anatol Blass, David Masiello, and Mauricio Coutinho.



Kevin Shuford (blue shirt) after his Ph.D. defense. Kevin is Jeff Krause's first student to defend.



*Back Row: Stig Flodmark, Gilda Loew, Frank Harris, Ruben Pauncz, Joop de Heer, Harrison Shull, Inga Fischer-Hjalmars, John Pople.
 Front Row: Arthur Frost, Roy McWeeny, Douglas McClure, Arthur Freeman, Eli Burstein, Per-Olov Lowdin*