QUANTUM THEORY PROJECT

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The Quantum Theory Project (QTP) is the world's largest academic group in computational and theoretical chemical physics and quantum chemistry.

Working across the traditional boundary between Physics and Chemistry is increasingly important for progress in nano-scale systems, molecular-scale biology, and new materials.
Quantum Theory Project

Departments of Chemistry and Physics

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QTP overcomes that barrier with:

✦ Dual appointments for faculty
✦ Teaching interdisciplinary graduate courses
✦ Members from both disciplines on graduate students committees
✦ Projects which provide a research opportunity for undergraduates
✦ Our large-scale computing laboratory
✦ The Sanibel Symposium
✦ External funding of over $1 million/yr

Institute for Theory and Computation in Molecular and Materials Sciences

11/5/2002
I am primarily interested in developing the theory and application of first principle electronic structure theory for molecules.

My group pioneered the development of coupled-cluster (CC) theory which now offers the reference results for most problems.

We also introduced \textit{ab initio} density functional theory and have generalized CC/MBPT for polymers.
Our interests include:

✦ Metastable molecules, like the unknown $N_4$, $N_5^-$, and $N_8$;

✦ NMR coupling constants across H bonds;

✦ Vibrational, Raman, photoelectron, electronic and ESR spectra;

✦ Modeling of materials using novel quantum chemical tools;

✦ Studies of interstellar species.

According to the Institute of Scientific Information, our work ranks among the most cited in chemistry.
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My research aims at development and application of computer-based theoretical methodologies for investigation of physical problems in complex systems.

The goal is to develop a basic understanding of physical and chemical properties of atomic and molecular clusters.

These systems exhibit unique properties because of their finite size, and therefore are of great fundamental significance as well as technological value.

Hai-Ping Cheng
Associate Professor
Physics

Institute for Theory and Computation in Molecular and Materials Sciences
We are working on systematic investigations of size-dependent energetic, structural, dynamic, and thermodynamic properties of various clusters, the interaction between clusters and the surface of bulk matter, and the transition from the atomic and molecular regime to the condensed phase.

In the last four years, we have focused on two major projects:

✦ the structure and dynamics of water clusters and
✦ particle-surface interactions.
I am responsible for operating the computing environment at QTP.

I teach a course in Advanced programming which discusses all issues involved in programming for scientific computing: including architecture of modern CPU's and parallel computers, object oriented design, correct programming (Fortran 95 is used as example language), debugging and performance analysis, message passing programming, and thread programming.
I use the development of a high performance, portable, parallel software library for quantum chemical integrals, called QTIP as testing ground for research and teaching of high quality software engineering.

Since 1986, my colleague Yngve Öhrn and I have developed the theory of the Electron Nuclear Dynamics (END). I am the principle author of the software package ENDyne implementing this theory. We have made several interesting studies which compare remarkably well with experiment.
The main focus of my recent research has been toward developing new or improved methods for making calculations of electronic structures and static or dynamic properties of molecules and extended systems.
Another theme among my research interests has been the use of symbol manipulation programs ("computer algebra") to develop computationally useful formulas for physical quantities when pencil-and-paper mathematics leads to unmanageable complexity.
Research in my group focuses on theoretical studies of time-dependent laser-matter interactions.

Advances in laser technology over the past few years have created a unique opportunity to study matter at its most fundamental level.
Laser pulses can now be produced on the time, length, and energy scales of atomic, molecular, and electronic motion.

This enables direct investigations of chemical systems as they are reacting and offers the possibility to move beyond the passive observation of materials to the active control of them.
Research in my group deals with theoretical and computational aspects of molecular and materials sciences, with emphasis on the unified treatment of physical and chemical kinetics using quantum molecular dynamics.

It includes collision-induced and photoinduced phenomena in the gas phase, clusters, and at solid surfaces.
Our aim is to provide a fundamental approach to molecular dynamics, where electronic and nuclear motions are consistently coupled to account for quantal effects.

We use quantum and statistical mechanics, mathematical, and computational methods, to describe time-dependent phenomena (such as femtosecond dynamics and spectra) in both simple and complex molecular systems.
A major area of my research is the design and development of the Colliding Beam Fusion Reactor (CBFR). In collaboration with Norman Rostoker, University of California, Irvine, we have designed the novel fusion reactor. It uses protons (p) and boron-11 (\(^{11}\text{B} \)) for fuel. Central to the design is the use of a so-called Field Reversed Configuration (FRC) plasma.
A multifaceted study is underway to establish the full feasibility of the design. Most of the large-scale calculations, theory development and nuclear polarization are centered in QTP, University of Nebraska, Lincoln, and UC Irvine. Experiments and engineering studies are being conducted at a start-up company, Tri-Alpha Energy, Inc. in Foothill Ranch, CA.
Modern experimental techniques using laser technology permit the study of molecular reactive processes, via time lapse photography as the reactants make their way towards products.

Theoretical methods in the time domain that can help to interpret such experiments have been developed in my research group under the name Electron Nuclear Dynamics (END).
The END equations take the form of coupled first-order differential equations in time and the dynamical variables whose time evolution are governed by these equations are the wave function parameters such as molecular orbital coefficients, nuclear average positions, and nuclear average momenta.

In this manner, electronic and nuclear dynamics are treated simultaneously and fully coupled.
My main interest relates to the modeling of biomolecules.

The complexity of their behavior and their obvious importance for life makes them fascinating systems to study.

The questions one can ask are almost limitless, and the recent sequencing of the human genome will bring the research in biophysics even more to the forefront.
I am particularly interested in the energetics and dynamics of peptides, proteins, and nucleic acids, as well as in the computational aspects of enzyme reaction modeling.

Current work involves the dynamics of the NO$_3$ anion in water. While one would expect this molecule to have a symmetric geometry with the three NO bonds being of equal length, our simulations show that the molecule prefers to break symmetry, creating a dipole moment and hence increasing its solvation energy.
Consider a beam of swift ions, from, for example, an accelerator, cosmic rays, or a reactor.

When the particles pass through matter, they interact with it, typically losing energy and causing some damage in the target system.

Such interaction is not wholly undesirable, as this is the method used to fabricate many microelectronic devices, run nuclear reactors, and to treat various tumors without recourse to the knife.
In other cases, the interaction leads to interference in communications, single event upset failures in computers, and radiation sickness in living things.

The details of the mechanism of the interaction of massive particle radiation with matter is thus of interest, and the understanding of these mechanisms and prediction of their effects on materials provides the unifying theme of my research, which is carried out in close collaboration with Yngve Öhrn.
My research focuses on predictive calculation of structures and properties of ultra-thin films and their crystalline counterparts, including fracture, quantum size effects, and high-pressure behavior of solids, development of algorithms for predictive simulations of materials, and of fundamentals of Density Functional Theory (DFT).
In the first category, we have recently completed a massive calculation on alpha-quartz using the Boettger-Trickey DFT Gaussian orbital code GTOFF. We now are exploring a different approach to potential fitting to first-principles results. This work is part of the NSF “KDI” project.

In the algorithm development category, we have been working on extending the algorithms in the GTOFF code to handle systems with 1D periodicity (currently it does 2D and 3D).
In the beginning of 2000, QTP was made aware of the possibility to acquire the Maui Supercomputer from the DoD High Performance Computing Modernization Program. That was the time when Beowulf clusters, built by assembling large numbers of PC's on racks became "the" thing to do. The name comes from the hero of a medieval poem: Beowulf was a fierce warrior who was going to defeat the dragon of the conventional "supercomputer".
Since we had the skills and expertise to run the Maui machine, a conventional "supercomputer" from IBM, we figured that we could get a lot of computing cycles even cheaper than with the Beowulf approach and the result would look prettier than PC's on shelves.

Thus we named our project after the legendary warrior princess Xena.
One year later, we heard about another super-computer becoming available, this time from Wright Patterson Air Force Base. We called this project Xena II. We had to work long and hard to get this system, but in August 2002 Xena II became operational in a new room, which was inaugurated on October 11, 2002.
Xena II is much more powerful than the Maui machine in many ways and more useful to a larger group of high performance computing users. We feel that our unique and unusual "Beowulf" strategy has been quite successful and invite you to visit our web site to learn more.
Visualization Lab

The lab was created in the Spring of 2001 with two major funding sources:

IBM Shared University Research award with matching funds from Physics, QTP, College of Liberal Arts and Sciences, and Office of Research and Graduate Education to Professor Hai-Ping Cheng as P.I. provided nine RS/6000 workstations.
Visualization Lab

NSF Major Research Instrumentation award to Professor Sam Trickey as P.I. and Professors Chris Stanton, Hai-Ping Cheng and Jeff Krause as co-P.I.’s with matching from Delta Airlines, Physics, Chemistry, QTP, College of Liberal Arts and Sciences, and Office for Research and Graduate Education provided the 3D ImmersaDesk visualization screen and the SGI Onyx 2000.
Guide Lines for Usage

The lab is for use by Physics and QTP researchers with a focus on simulation of clusters, surfaces, and large molecules and on visualization of such systems.

The lab can also be used for training and advanced classes on simulation and programming methods.
The Nuts & Bolts
The Visualization Lab Hardware

The lab has a simulation and visualization cluster of 9 work-stations, thus 18 people can be trained in one session.

6 IBM RS/6000 42P model 270 workstations with four 375 MHz POWER3 processors, 3 GB of RAM and 38 GB of disk. Each station has a high 3D graphics card and 19” monitor.

3 IBM RS/6000 42P model 170 workstations, each with a 375 MHz POWER3 CPU and 256 MB RAM and 18 GB disk. Each workstation has a 3D graphics card and 19” monitor.
The second part of the lab’s equipment is a 4 CPU SGI Onyx 2000 with 8 GB RAM and 45 GB disk space with a FakeSpace ImmersaDesk attached to it. It allows up to 5 people to be immersed in a virtual scenery in front of the ImmersaDesk.
The Visualization Lab Software

- SGI Onyx2:
  Visualization:
  VIMD,
  OpenDX

Compilers:
  f77,
  f95,
  C,
  C++
The Nuts & Bolts
The Visualization Lab Software
- IBM 42P-270 and 42P-170:
  Visualization:
  VIMD, OpenDX
  Compilers:
  f77, f95, C, C++, gcc, g++
  Software development:
  Python, Tcl, MPI
  Various:
  Gaussian 98

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The Xena I cluster has 134 nodes, 9 of which are for interactive use. Each node has a 33 MHz POWER2 CPU and 64 MB or 128 MB of RAM.

About half the nodes have a one GB local disk.

The other half use a disk on our main server.

All nodes are connected by an 40 MB/sec full duplex High Performance switch.
The XENA II system has
✦ 192 nodes, each with:
✦ 135 MHz POWER2SC CPU,
✦ 1 GB of RAM and
✦ 9 GB of disk space.

All nodes are connected by a 150 MB/sec full duplex, redundant path SP switch. The system has 420 GB of global storage consisting of 192 2.2 GB disks on 16 SSA controllers made available to each node through the SP switch as a GPFS (general parallel file system).
The Nuts & Bolts
Configuration of Xena III

The system has 127 nodes each with:
- 160 MHz POWER2 Super Chip CPU,
- 512 MB RAM, 9 GB disk,
- 150 MB/sec SP Switch.

The system has 1.4 TB of global SSA disk storage in 3 racks with 20 drawers, each with 16 4.5 GB disks accessible through 16 SSA 80 MB/s adapters.
Upcoming Events

2003 Pan American Workshop
Cuernavaca, Mexico
February 17-19, 2003

✦ Promote scientific contacts among scientists in the US, Latin America, Canada, and the Caribbean;

✦ Develop theoretical and computational methods applicable to problems of common interest in the molecular and materials sciences;

✦ Encourage long term collaborations with those scientists as they return to their countries.
Upcoming Events

43rd Sanibel Symposium
St. Augustine, Florida
February 22-March 1, 2003

Focuses on forefront theory and computation in:

✦ Quantum chemistry,
✦ Condensed matter physics,
✦ Molecular dynamics,
✦ Quantum biochemistry,
✦ Quantum biophysics

“Hands-on” Workshop focusing on computer applications for simulations for Graduate and advanced Undergraduate Students.