In modeling complex materials and their interfaces, it is often necessary to take account of the dynamics of a large number of atoms and electrons. Problems of this kind arise, for example, in such diverse fields as magnetism, corrosion science, electrochemistry, polymer science, and biology. One approach to this problem is a direct dynamics calculation in which the equations are solved for the electronic structure at each step in the classical evolution of the positions of the atomic nuclei of a large system.

Supercomputing Institute Fellow Professor J. Woods Halley (Physics and Astronomy) and his research group are developing a version of this approach that is suitable for transition metals, or materials involving them; this approach is computationally tractable for complex systems. The basic idea is to use the same kind of first principles electronic structure calculation (i.e., a plane wave local density approximation calculation) that is used in the Car-Parrinello method to parametrize a simpler version of the electronic structure problem—self-consistent tight binding molecular dynamics; this kind of calculation is not as expensive to solve at each step in an atomic dynamics. The term “self-consistent” refers to Hartree self-consistency, familiar from the well-known Hartree and Hartree-Fock approximations. The self-consistent aspect distinguishes this method from the original tight-binding and extended Hückel approaches. Electronic properties of the isolated ions of the constituent atoms of the material being simulated are directly incorporated into the model from

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experiment and cause the on-site energies of the ions in the model to depend on the total number of electrons on the ion. In this way, the difficult problem of the local electronic structure around an atom does not have to be solved repeatedly while studying many-atom systems.

Patrick Schelling, now at Argonne National Laboratory, developed many aspects of this approach in his thesis while with the Halley group. He applied it to the study of rutile titanium dioxide surface structure and polaron structure in rutile titanium dioxide, to grain boundaries in rutile, and to titanium metal-titanium dioxide interfaces.

As a methodological test bed, titanium dioxide has the advantages of relatively simple structure, no magnetic effects, and abundantly available experimental and first principles calculational information. TiO$_2$ is also an important material for engineering applications; it has a very large dielectric constant, and its properties at microwave frequencies are exploited in microwave devices. Many of its close cousins, the perovskite titanates, are ferroelectric.

Stoichiometrically pure titanium dioxide is an insulator, but if, as is usually the case, it is somewhat oxygen deficient, it self-dopes with electrons and is an $n$-type semiconductor. Because the dielectric constant of the material is very large, the carriers are not believed to propagate like free electrons but are surrounded by a cloud of lattice distortion that increases the effective carrier mass significantly. Such a combination of electron-plus-lattice distortion is called a polaron. Theories of polaron structure and dynamics go back to the 1950s; however, there are very few detailed calculations of the properties and structure of polarons in specific materials. Schelling first fit the tight binding molecular dynamics model of rutile to first principles calculations of the electronic structure of stoichiometrically perfect TiO$_2$ (using, for the first principles calculations, codes developed in the research group headed by Institute Fellow James...
Chelikowsky, who is Professor of Chemical Engineering and Materials Science at the University of Minnesota). Schelling then used the model to study the structure of polarons in it by adding an extra electron to a structure during a molecular dynamics calculation in which the electronic structure was redetermined self-consistently after each atomic step. These calculations were more detailed than previous polaron calculations and focused on a higher temperature regime in which the atomic motions could be treated as classical. A surprising result was that the electronic wave function associated with the added electron was localized throughout the finite-temperature simulations. The localization, which became less pronounced at lower temperatures, was interpreted as caused by the thermal disorder of the atoms around the carrier.

To understand how titanium dioxide protects titanium metal from corrosion, one needs to model the titanium/titanium dioxide interface. Schelling was able to show that first principles results for the cohesive energy and band structure as function of volume per unit cell of titanium metal could be rather well reproduced with the self-consistent tight binding methods. These calculations were carried out with new “order N” techniques in which the computational effort scales linearly with the number \( N \) of atoms in the system.

He placed samples of titanium metal and titanium dioxide in proximity and allowed the atomic positions to relax to equilibrium (at zero temperature). At the same time, he recalculated the electronic structure after each step in which the atoms relaxed along the forces determined from the electronic structure as calculated in the preceding step. A striking result is that Friedel oscillations of the charge in the metal have been induced on the metal side of the interface (as shown in the figure on page 2).

These preliminary results on interfaces are exciting because they open the way to study of a variety of technically important Schottky barrier interfaces in microscopic detail.

Recently, Min Zhuang, a research associate in the Halley research group, has been extending these methods to take account of the effects of electronic spin. The basic idea is to take account of the fact that the electronic structure of the constituent ions of a solid or liquid is governed by Hund’s rule, which states roughly that, other things being equal, the electronic spin of an ion will be maximized. To systematically take this into account in the self-consistent tight binding model, the on-site energies of the model are caused to depend both on the charge of the ion and on its total spin. Then, both the charges and the spins of the ions are self-consistently determined in the electronic structure calculations.

To test the method, Zhuang has made calculations on rutile MnO\(_2\), MnF\(_2\), and on the spinel structure LiMn\(_2\)O\(_4\). The latter is of interest as a cathode material for advanced lithium polymer batteries. Zhuang has shown that the method predicts the well known antiferromagnetic structure of MnF\(_2\), including the correct magnetic moment per ion, within a few percent. In the case of MnO\(_2\), he finds spin spiral structures quite similar to tentative reports in the experimental literature on this material. These results suggest the possibility of predicting microscopic magnetic structures using these methods.

Other members of the Halley research group are working on the application of these methods to water, to other transition metal oxides, and to noble metals.
Detailed chemical kinetics models of complex reactive systems are large-scale mathematical models that combine lengthy lists of elementary chemical reactions (the reaction mechanism) with transport for an accurate description of process chemistry and rates of transformation. The models are suitable for many purposes; for example, they are used to describe reactive flows such as those encountered in the chemical process industry, or to better understand combustion or environmental chemistry.

Supercomputing Institute Associate Fellow Robert W. Carr, who is Professor of Chemical Engineering and Materials Science, and his group of researchers are focusing on the development of models for chemical vapor deposition and for atmospheric chemistry. The use of supercomputers, the development of efficient numerical algorithms, and advances in the kinetics of elementary reactions and in computational chemistry, all contribute to progress in the development of detailed chemical kinetics models.

Chemical vapor deposition (CVD) is a process for depositing thin films on solid surfaces by flowing a molecular source of the elements to be deposited over a heated substrate in a cold-walled reactor. The source is commonly a vapor and the substrate temperature is frequently about 1000 K. In the hot region, thermal decomposition of the source species occurs both on the surface and in the adjacent gas phase. Reactive intermediates adsorb on the surface where reactions leading to film growth take place. Accurate description of this chemistry requires tens to hundreds of elementary chemical reactions. The development of mathematical models for CVD reactors has advanced to the point where it is possible, with supercomputers, to compute the flow and temperature fields for almost any reactor configuration of interest. However, computation of film growth rates and material properties is still in an embryonic state because of gaps in knowledge of the kinetics and mechanisms of the gas-phase and surface chemistry occurring during deposition.

Mechanism development consists of a mix of experimentation, literature searching, and application of theory. When literature data cannot be found, key reactions must be studied experimentally to obtain accurate values of rate coefficients. Other reactions can be investigated by the methods of computational chemistry, and some relatively unimportant ones can be treated by empirical means. One of the reactions in the GaN deposition system the Carr group recently investigated is the formation of the Lewis acid-base pair between trimethylgallium and ammonia. This reaction is thought to inhibit GaN deposition, but there was a scarcity of reliable data. Measuring the equilibrium constant as a function of temperature, the group found the enthalpy of reaction to be -15.2 kcal mol\(^{-1}\).

\textit{Ab initio} quantum chemistry calculations on the reactant and the product yielded an enthalpy of the reaction of -15.9 kcal mol\(^{-1}\), in good agreement with experiment. With the energetics of the reaction firmly established, the researchers have been using the theory of unimolecular reactions to get an estimate of the rate coefficient for unimolecular dissociation of the adduct. Application of microscopic reversibility then gives an estimate of the rate coefficient for the association of trimethylgallium and ammonia. These \textit{ab initio} calculations revealed the appropriate levels of theory for reliable estimation of the energetics of organogallium compounds.

This experience has allowed the group to calculate good estimates of the rate coefficients for successive unimolecular elimination of each of the three methyl radicals from trimethylgallium.
The decomposition of trimethylgallium may be the rate limiting step in GaN deposition, in which case it will be important to know the decomposition rate completely.

Another area of study is the atmospheric chemistry of halogenated species, including replacements for the ozone-depleting chlorofluorocarbons. These compounds are present in the atmosphere in trace amounts, and can be removed through a multistep oxidative degradation process in which free radical intermediates play a role. Among these are halogenated alkoxy radicals, species whose reactivity is not well understood, and which are frequently a stumbling block in attempting to understand the oxidative degradation chemistry. The group has been using time-resolved mass spectrometry to investigate the kinetics of some halogenated alkoxy radicals. The experimental method is limited to studies at pressures of a few torr to 40 or 50 torr, and temperatures that typically are higher than the approximately 200 K minimum that is found at the troposphere-stratosphere boundary. The radicals being studied are unstable, undergoing unimolecular decomposition with pressure and temperature dependent rate coefficients. To determine rate coefficients over the full range of atmospheric pressure and temperature, ab initio calculations of the decomposition energetics are being performed, the results of which can be used in conjunction with the theory of unimolecular reactions to calculate the rate coefficients. Matching the calculations with experimental data ensures reliable values of the rate coefficients over the entire temperature and pressure range. Figures 1–3 show transition states for Cl-atom and HCl elimination from the chloromethoxy radical. The Carr group recently computed these structures using G2 and G2(MP2) theories on the IBM SP.

Figure 1: Chloromethoxy radical

Figure 2: Transition state of Cl elimination

Figure 3: Transition state of HCl elimination
The Supercomputing Institute for Digital Simulation and Advanced Computation hosted a gathering of scientists from around the world in a two-day workshop on Excited State Properties and Response Functions for Materials on November 13–14, 2000. Co-sponsored by the Computational Materials Sciences Network (CMSN) of the Department of Energy and the Supercomputing Institute, the workshop provided a forum for the growing international community of researchers in this field, many of whom presented their work in talks and discussion groups.

Excited state physics is a challenging new field, derived from the many experimental probes of materials properties, which involve electronic excitations. Modern high intensity photon sources (synchrotrons, ultrafast lasers, etc.) can now probe materials with unprecedented resolution and open the potential for novel materials processing and materials science studies. In the last few decades, computational physics has achieved enormous successes in describing ground-state properties. In contrast, quantitative descriptions of excitations and response functions are just emerging.

The objective of the workshop was to assess the technical and computational issues that will enable calculations of linear and nonlinear response functions at the same level of sophistication and accuracy that is now possible for the ground-state. Specific short- and long-term objectives that will impact theoretical understanding and applications to materials studies, including characterization and processing, were discussed and presented at this meeting, as described below.
The workshop began with a series of welcoming remarks by James R. Chelikowsky (University of Minnesota), Manfred Leiser (U.S. Department of Energy), and John Rehr (University of Washington).

Following these opening comments, Lars Hedin (Lund University) began the first session of the day on fundamental theory with his talk, “A Model Based on the GW Theory and Its Use Beyond Quasi-particle Energies.” Steven G. Louie (University of California–Berkeley) continued on this theme, speaking on “Electron-hole Interaction and Optical Excitations.”

The next session was devoted to experimental processes and applications. Franz Himpsel (University of Wisconsin at Madison) discussed “Exotic Excited States in Low-dimensional Systems and in Nanostructures.” John Rehr (University of Washington) spoke on “Applications of Excited State Theory to Synchrotron X-ray Spectroscopies.”

The afternoon sessions began with the topic of electronic excitations and time dependent phenomena. The first speaker in this session was Lucia Reining (École Polytechnique, Palaiseau, France), whose talk was entitled “The Calculation of Electronic Excitations: Some Recent Developments.” James R. Chelikowsky (University of Minnesota) then spoke on “Time Dependent Density Functional Theory (TDDFT) for Confined Systems.” Finally, to conclude this session, Sokrates Pantelides (Vanderbilt University) spoke on “Core Excitation Spectra.”

The second afternoon session was devoted to experimental processes and electron correlation. Lorin Benedict (Lawrence Livermore National Laboratory) opened the session with

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his discussion of “Excited State Properties of Materials in Extreme Conditions.” Eric Shirley (National Institute for Standards and Technology) continued this theme in his talk, “Some Computational Developments in Core and Valence Excitations.” The day concluded with a general discussion and several break-away meetings on specific topics.

The second day of the workshop was structured to address the research of many of the participants. John Wilkins (The Ohio State University) led off with a summary of his work on “GW and III–V Offsets.” Andrew Canning (Lawrence Berkeley National Laboratory/National Energy Research Scientific Computer Center) presented an update on his institutions’ progress in the field and their recent activities. George Bertsch (University of Washington) provided a comparison of time dependent density functional theory (TDDFT) methods, while Serdar Öğüt (University of Minnesota) discussed his work: “Ab Initio Calculations for the Dielectric...
This was followed by Sohrab Ismail-Beigi (University of California–Berkeley), who discussed “Gauge-invariant Coupling of Non-local Potentials to Electromagnetic Fields,” and Mei-Yin Chou (Georgia Institute of Technology), who has been considering “Quasi-particle Calculations for Metal Hydrides.”

Following a short break, more short reports were presented: Igor Vasiliev (University of Illinois) described his work on the time dependent local density approximation applied to nanoclusters; Kevin Leung (Sandia National Laboratory) discussed GW calculations on simple models; and Michel Van Hove reported on “Full-potential and Core-hole Effects in Photoelectron Diffraction.” The workshop continued with a presentation by Warren Pickett (University of California–Davis) on “Crystal Field Excitations from Local Density Approximation (LDA) + U Total Energy Differences,” and by John Shumway (NREL): “Quantum Monte Carlo Calculations of Exciton Systems.” Wai-Yim Ching (University of Missouri at Kansas City) presented a discussion of his recent work: “Inclusion of the Core-Hole Interaction in the X-ray Absorption Near Edge Structure (XANES)/Energy Loss Near Edge Structure (ELNES) Spectra of Oxides and Nitrides.” The final presentation of the workshop was given by Dilano Saldin (University of Wisconsin at Milwaukee).

The workshop concluded with an afternoon session of discussion and planning, including team reports, organization of next year’s workshop, and other discussions.
This summer, ten undergraduate student researchers from across the country served ten-week internship appointments at the Supercomputing Institute; these included four students in the Computational Neuroscience Program. The students were selected from a pool of 58 applicants. The students worked closely with faculty advisors on diverse projects, many of which were related to their present or possible future areas of research interest.

The Supercomputing Institute Summer Internship Program, currently in its tenth year, promotes undergraduate involvement in ongoing and new research. Areas of study include scientific computing, digital technology, visualization in the physical, medical, and social sciences, and engineering, as well as in new software development efforts for scientific computing and graphics support for such projects. The main goal of the program is to carry out useful and interesting research. This program provides an opportunity for a challenging and enriching educational experience for undergraduate students interested in pursuing graduate or professional education and research in scientific computing and/or graphics.

During the summer, interns participated in Institute-sponsored tutorials specific to high-performance computing. To conclude the summer, the interns presented talks open to the entire research community. These talks allowed them to share their work and to gain experience making scientific presentations. The program allowed the students to perform research in close collaboration with faculty investigators and their research groups, and to discuss research with faculty members, postdoctoral associates, graduate students, and other interns with similar interests.

**Project Descriptions**

**Aron Cooper**, a major in Aerospace Engineering and Astrophysics at the University of Minnesota, worked with Dr. Shri Ramaswamy (Wood and Paper Science). Using MATLAB, he wrote programs to reconstruct as a 3-dimensional matrix the images of the porous media taken in the xy-plane. From these reconstructions, Aron was able to analyze samples in the xy-, yz-, and xz-planes. Aron's own code, based on functions found in
MATLAB, was used to produce skeletonized images of every slice in all three planes. With these he attempted to extract data which would allow him to characterize the porous structure in each plane in terms of mass transfer, heat transfer, and permeability. His findings revealed that porous structure is very similar in the xz- and yx-planes, and that the structure in these planes does in fact vary enough from the xy-plane for one to expect a substantial difference in heat transfer, mass transfer, and permeability.

Majoring in Biochemistry and Quantitative Methods in the Computer Science Department at the University of St. Thomas, Loren Gragert worked with Dr. Germana Paterlini (Pharmacy). He concentrated on two different areas: in one, he performed homology modeling simulations (an increasingly important tool in proteomics) to construct the loop and C-terminal regions of the chemokine receptor CCR5, the major co-receptor for HIV-1 entry into macrophage cells. In the second area, he modeled a dimyristoylphosphatidylycerol (DMPC) lipid bilayer for use in simulations involving membrane embedded proteins. The computational model of CCR5 will aid investigations into the mechanism of binding of chemokines, small molecule antagonists and the gp120 envelope protein of HIV-1. This work complements modeling of the DMPC bilayer, which will be useful in simulating membrane-embedded proteins in their physical environment.

Nicholas Koshnick, a major in Physics at Dartmouth College, worked with Professor J. Woods Halley (Physics and Astronomy). Focusing on the development of a tight binding code for titanium dioxide (see story on page 1 of this Bulletin), Nicholas used extra (S and P type) orbitals, included with titanium atoms, in order to describe a stable oxygen vacancy while correctly accounting for their interactions. Beyond this, Nicholas attempted to insert the resulting changes into a titanium dioxide-titanium interface code.

Describing his research, Loren Gragert presents techniques in homology modeling simulations, such as those he produced during his internship.

Aron Cooper outlines his research findings to his faculty advisors and fellow interns.

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By making several small improvements to an existing description of S and P orbitals in a titanium code, Nicholas and his research team constructed a code that described stable oxygen vacancies in titanium dioxide. Nicholas also parameterized parts of the titanium interactions to achieve a better description of the process.

Andrea Lay, a student from Tulane University majoring in Biomedical Engineering, worked with Dr. David D. Thomas (Biochemistry, Molecular Biology, and Biophysics). Her topic of study was the simulation of electron paramagnetic resonance (EPR) spectra from molecular dynamics trajectories. Utilizing EPR spectroscopy to study the rotational dynamics of muscle proteins during muscle relaxation and contraction, Andrea sought to understand the mechanism of muscle contraction itself. Prior to this research, many computer programs had been written to simulate spectra based on a rigid orientational distribution or general rotational motion models; however, very little work has been done on the simulation of spectra corresponding to specific rotational motions predicted from high-resolution structural data and molecular dynamics simulations based on high-resolution protein structural data. Andrea wrote a program to simulate these spectra, basing her work on the Hamiltonian equation and the research of several former lab members, including a simulation program that accounted for the rigid limit of the probe.

Peter Oman, a University of Minnesota student who is majoring in Mathematics and Chemistry, worked with Professor Darrin M. York (Chemistry) and focused his research on a molecular simulation of the HIV-1 nucleocapsid protein bound to SL3 RNA. Since the HIV NC protein is virally encoded, consisting of two CCHC-type zinc knuckle arrays connected by a small linker sequence, and is
therefore involved in virtually every stage of the HIV life cycle, it is a crucial component in the study of HIV in general. Peter’s goal in his own work was to obtain a detailed dynamical picture of the HIV NC-RNA interactions at the atomic level, and to characterize the role of zinc ions on the structure and binding processes. To this end, he carried out simulations using the new CHARMm 27 all-atom force field, designed for accurate simulations of nucleic acids and proteins. An initial model was constructed based on the NMR solution structure of NC bound to the third stem-loop on the psi-recognition site of the genomic RNA with amino acids in their characteristic protonation states at neutral pH.

A Stanford University Psychology and Pre-Med major, David Joseph Regelmann worked with Dr. William B. Gleason (Laboratory Medicine and Pathology Department), performing computational studies of vascular endothelial growth factor VEGF. David initially used the program LIGPLOT to study the interaction of a number of sulfated polysaccharide complexes with proteins of known three-dimensional structure. LIGPLOT analyzes intermolecular distances to characterize hydrogen bonding and other interactions between the ligands and proteins. He then began work on models suitable for molecular mechanics and dynamics studies of the interaction of VEGF160 (a heparin-binding isoform) with heparin model compounds. Parallel experimental studies using X-ray crystallography will also be aided by the availability of his model structures.

As a major in the Integrated Science Program in the Department of Mathematics at Northwestern University, Matthew Salomane worked with Drs. Heinz G. Stefan (St. Anthony Falls Laboratory) and Vaughn Voller (Civil Engineering Department) on the observation of dissolved oxygen dynamics in a vegetated lake. Matthew designed, coded, and tested a deterministic model describing the seasonal growth and dissolved oxygen dynamics of aquatic macrophytes in lakes. The model was based on general information provided by his advisors, Drs. William Herb and Omid Mohseni. Special attention was paid to the role of the plants’ self-shading in creating a larger-than-expected oxygen deficit near the sediment. During his internship, Matthew spent one day at Holland Lake in Eagan, Minnesota, obtaining samples of lake weeds for photography and classification, as well as taking lake temperature and oxygen measurements. These projects provided Matthew with valuable experience in the formulation and

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design of a mathematical model, as well as insight into the ways models can be used to solve problems in the wider scientific arena.

Nathan Shultz, majoring in Chemistry at St. John’s University and the College of St. Benedict, worked with Professor Donald G. Truhlar (Chemistry). The bulk of his research explored possible ways of increasing the accuracy and efficiency of electronic structure calculations for problems involving chemical kinetics. The approaches studied were the use of Multi-Coefficient Correlation Methods as an alternative to the slow convergence of traditional \textit{ab initio} electronic structure calculations and Hybrid Density Functional Theory with parameters adjusted for kinetics.

Sundeep Shakya, a University of Mississippi student majoring in Computer and Information Science, worked with Professor Christopher W. Macosko (Chemical Engineering and Materials Science), under the co-supervision of Russell Hooper, with emphasis on using adaptive re-meshing in large strain drop simulations. Sundeep focused on developing a remeshing feature to allow the simulation of much larger drop deformations. This required a robust three-dimensional meshing algorithm that could generate a domain mesh from an active surface mesh and could be run in batch mode. Since writing such an algorithm would take much time and effort, and since several commercial mesh generators already exist, the researchers decided to choose from among the various generators available at the Minnesota Supercomputing Institute in order to find the one that best fit with their requirements. GAMBIT was tried and found to be insufficient for the project at hand, so Sundeep finally decided to use HYPERMESH, as it provided the most straightforward means of interfacing with the existing finite element (FEM) code. Sundeep also wrote a program in C to execute HYPERMESH in batch mode after each time step in the droplet deformation simulations.

Andrew Watson, a major in Computer Science at the University of Minnesota, worked with Professor Leonard J. Banaszak (Biochemistry, Molecular Biology, and
Biophysics) worked on setting up new computer system administration duties in a dedicated computational biology laboratory. The system involves a collection of Pentium III computers in a Linux/Windows NT dual-boot environment, and multiple software packages were installed on the machines. Andrew worked out the protocols for the desired Linux configuration, and he coded multiple c-shell scripts in the process of configuring Linux and making the system recoverable. This activity included obtaining system recovery scripts and making a drive-mounting script that would execute on login. Andrew also wrote multiple scripts in Windows NT and installed software programs such as S.P.O.C.K., O, CrystalClear, and CNS-Solve.

**Computational Neuroscience Program**

In the Computational Neuroscience Program, selected undergraduates worked on projects with faculty in an interdisciplinary program co-sponsored by the National Science Foundation. Research in this field requires the use of quantitative methods and computer-related analysis techniques to study the development, structure, biochemistry, and function of the nervous system.

**Pedro Gautier** (Chemistry, Universidad Metropolitana, Bayamon, Paraguay) and **Daniel Melendez** (Natural Sciences, Universidad Metropolitana, Bayamon, Paraguay) worked with Professors Darrin M. York and Jiali Gao (Chemistry) during their internship. Their project used computational chemistry to model organic reactions.

**Corey Maley** (Computer Science, Mathematics, Psychology & Philosophy, University of Nebraska–Lincoln) worked with Professor Linda M. Boland (Neuroscience).

Under the guidance of Professor Boland and Dr. Anthony Varghese (Washington Avenue Bridge Postdoctoral Fellow), he used C++ to construct a model that can be used to simulate the firing of CA3 hippocampal pyramidal neurons. The model can be helpful both in testing predictions and in designing physiological experiments.

**Timothy Sonbuchner** (Biochemistry, Biology, & Mathematics, Gustavus Adolphus College) worked with Professors Christopher J. Cramer and Donald G. Truhlar (Chemistry), and Washington Avenue Bridge Postdoctoral Fellow Dr. James Xidos. Timothy worked on deriving accurate partial atomic charges for use with quantum mechanical solvation models. This is the first step in the development of specialized versions of these models for applications to neurotransmitters and other biomolecule interactions.
Each year, the Supercomputing Institute provides grants for research scholarships for supercomputing researcher at the University of Minnesota. During 2000–01, the Supercomputing Institute provided seven research scholarships to research associates who work closely with Supercomputing Institute principal investigators.

**Anguang Hu**, Department of Chemistry, University of Minnesota, is working with Professor Darrin M. York of the Department of Chemistry on an integrated parallel linear-scaling FORTRAN-95 (F95) electronic structure package. This involves integrating numerical and solid harmonic Gaussian density-functional methods, new pseudopotential techniques, and d-orbital semiempirical models. The program serves as a modularized F95 software platform for future modifications, including extension to plane-wave basis functions, and a seamless interface with their new molecular simulation codes. The former is used as a convenient departure point for the development of new nonlocal functionals for the exchange-correlation energy in density-functional theory and the latter is used a framework for performing new hybrid quantum mechanical and molecular mechanical (QM/MM) methods using the polarizable force fields being developed in their group.

**Bijaya Karki**, Department of Chemical Engineering and Materials Science, University of Minnesota, has been working with Professor Renata M. Wentzcovitch (Chemical Engineering and Materials Science and Supercomputing Institute Associate Fellow) on first-principles computer simulations to study the thermoelastic properties of the silicates and oxides (MgSiO$_3$, CaSiO$_3$, MgO, CaO, Al$_2$O$_3$, SiO$_2$, and their high-pressure polymorphs) that are generally considered as the major constituents of the Earth’s mantle. The methodology used is based on the density
Leeor Kronik, Department of Chemical Engineering and Materials Science, University of Minnesota, has been working with Professor James R. Chelikowsky (Chemical Engineering and Materials Science, and Supercomputing Institute Fellow). Dr. Kronik—who came to the Chelikowsky Group following a position as research associate at the Department of Electrical Engineering, Tel Aviv University—has taken part in developing numerical algorithms to describe and predict the properties of complex systems such as atomic clusters. These systems often resemble neither atomic-like or bulk-like systems. As such, they are of considerable interest in terms of technological applications (e.g., nanoscale devices) and fundamental science (e.g., the role multiscale phenomena play in spanning systems from the atom to the crystal). State-of-the-art quantitative predictions of important parameters such as inter-atomic distances, static polarizabilities, and optical excitations often rely on all-electron approaches, and the computational demand of such studies imposes severe limitations on the size of the cluster that can be studied. Dr. Kronik is utilizing a different method, one devised in part by Professor Chelikowsky’s group. In this method, *ab initio* pseudopotentials are constructed within the framework of a gradient-corrected density functional and a finite-difference real space approach is used to solve for the electronic properties of the system. This approach allows researchers to make accurate predictions of important parameters such as inter-atomic distances, static polarizabilities, and optical excitations.

Leeor Kronik works with Professor James Chelikowsky to develop numerical algorithms to describe and predict the properties of complex systems such as atomic clusters.

Dr. Ilaria Perugia works with Professor Bernardo Cockburn on the simulation of the rheological properties of magneto-rheological fluids.
predictions of cluster properties at a fraction of the computational effort of all-electron calculations. It also allows one to include the role of temperature via *ab initio* molecular dynamics simulations. Dr. Kronik has discovered that discrepancies between the calculated polarizabilities of alkali metal clusters and experiment is largely due to the neglect temperature effects. This work resolved a puzzle in the literature that has existed for the last ten years.

Ilaria Perugia, from the Dipartimento di Matematica, Università di Pavia, Pavia, Italy, is working with Professor Bernardo Cockburn (Mathematics, and Supercomputing Institute Fellow) on local discontinuous Galerkin (LDG) methods for non linear mathematics. The LDG methods are locally conservative, high-order accurate methods; they allow for greater flexibility in adaptive algorithms since no inter-element continuity must be enforced. Dr. Perugia's main application is the simulation of the rheological properties of so-called magneto-rheological fluids. These fluids have many magnetizable particles in suspension, and these particles change the rheological properties of the fluid when it is subjected to magnetic fields. Computation of the magnetic field of the whole fluid by means of an iterative method will take place in two ways: (1) Given the magnetic potential at the border of the particles, a multipole technique is being used to compute the magnetic field in the fluid; with this information, they can compute the magnetic flux at the boundaries of the particles, and then (2) use their LDG method to solve for the magnetic field inside the particles in parallel.

Jeffrey Potoff, Department of Chemistry at the University of Minnesota, worked with Professor J. Ilja Siepmann (Chemistry, and Supercomputing Institute Fellow) on the development of non-polarizable and polarizable force fields for vapor-liquid equilibrium calculations. Thanks to recent advances in Monte Carlo simulation methodologies, the termination of vapor-liquid phase coexistence properties for a given model system has become more straightforward. The main limitation in the application of molecular simulation techniques for the calculation of phase diagrams for pure components and mixtures of real molecules stems from the lack of accurate, but computationally efficient, intermolecular force fields. In this project, Dr. Potoff developed accurate force fields for water, aldehydes, ketones, and amines, which are all chemicals that are important to a wide range of industrial processes. Mixture calculations were performed to assess whether additional factors, such as polarizability, are needed in order to be able to determine mixture vapor-liquid equilibrium data that are in quantitative agreement with experiment. Furthermore, Dr. Potoff performed calculation of the critical parameters for recently introduced polarizable water models.

Pavel Bělík, from the School of Mathematics at the University of Minnesota, works with Professor Mitchell B. Luskin (Mathematics, and Supercomputing Institute Fellow) on computational tools for microscale biomedical devices. With the intent of developing large-scale computational methods for the design of new active thin films, which will
have applications as micromachines and actuators, Dr. Bělík focuses his research on magnetostrictive and shape memory materials. Also, his research considered the application of a recently discovered class of active materials that combine shape memory and ferromagnetism. The challenges to this research are found in the presence of microstructure in the films which require innovative new computational techniques. The first stage of this work involved the development of computational models for simple micromachines such as valves and pumps based on magnetostrictive and shape memory materials. Such valves and pumps have been proposed for drug delivery systems in the human body to enable the application of strong medicines with short lifetimes directly to an affected area, in contrast to the application of weak medicines to the whole body at uniform concentration.

**Witold Dzwinel**, from the Institute of Computer Science, A.G.H., Krakow, Poland, is working with Professor David A. Yuen (Geology and Geophysics, and Supercomputing Institute Fellow) on using discrete particle methods for simulating cross-scale phenomena with reactions. Dr. Dzwinel is employing discrete-particle methods for studying chemical reactions in complex binary and ternary fluids in the mesoscale, spanning from hundreds of nanometers to microns. Both exothermic and endothermic reactions at various temperature and pressure conditions are being studied with a two-level approach involving both molecular-dynamics and dissipative-particle dynamics techniques. The outcome of this work will have a direct bearing on many different areas, spanning from reaction-diffusive flows in chemical geological sciences and to colloids.

**Dr. Pavel Bělík (right)** works with Professor Mitchell Luskin. They are developing large-scale computational methods for the design of new active thin films.

**Dr. Witold Dzwinel (right)** works closely with Professor David Yuen and the Yuen Research Group.
The 34th Annual Midwest Theoretical Chemistry Conference (MTCC) is being held October 5–6, 2001, at the University of Minnesota in Minneapolis. For the first Midwest Theoretical Chemistry Conference of the new century, the conference organizers have adopted a format consisting of talks by senior scientists (faculty and senior researchers at government laboratories and in industry) and poster papers by senior scientists, postdoctoral associates, and students.

The following is a list of the senior scientists who have committed to giving plenary presentations and their titles:

• Daniel M. Chipman, University of Notre Dame, “Reaction Field Theory for Electronic Structure”
• Christopher J. Cramer, University of Minnesota, “New Developments and Applications of SMx Models”
• Larry A. Curtiss, Argonne National Laboratory, “Computational Thermochemistry Using Gaussian-3 Theory”
• Ernest Davidson, Indiana University, “A Computational Verification of the Relation of Dyson Orbitals to Kohn-Sham Orbitals”
• Michael Davis, Argonne National Laboratory, “Geometric Approach to Multiple-Time-Scale Kinetics”
• Janet Del Bene, Youngstown State University, “NMR and IR Properties of Hydrogen-Bonded Complexes”
• Jerry R. Dias, University of Missouri at Kansas City, “Unified Structure Theory of Benzenoid Hydrocarbons”
• Clifford Dykstra, Indiana-Purdue University at Indianapolis, “Slipperiness on Sticky Intermolecular Interaction Surfaces”
• Karl Freed, James Franck Institute, University of Chicago, “IVO-CASCI Method as a Replacement for CASSCF Calculations in Electronic Structure Packages”
• Jiali Gao, University of Minnesota, “Combined QM/MM Simulations of Enzymatic Reactions and Membrane Proteins”
• J. Daniel Gezelter, University of Notre Dame, “A Reductionist Model for Biological Membranes”
• Rainer Glaser, University of Missouri at Columbia, “Theoretical Studies of DNA Base Deamination”
• Mark Gordon, Iowa State University, “Excited State H-Transfer Reactions”
• Stephen Gray, Argonne National Laboratory, “Real Wave Packet Approach to the Quantum Dynamics of Four-Atom Systems”
• Christopher M. Hadad, The Ohio State University, “Conformational Analysis of Carbohydrates Containing Arabinofuranosyl Rings”
• Lawrence B. Harding, Chemistry Division, Argonne National Lab, “Radical-Radical Recombination Reactions”
• William Hase, Wayne State University, “Dynamics of Central Barrier Crossings in Gas Phase X⁻ + CH₃Y SN₂ Nucleophilic Substitution Reactions”
• Katharine Hunt, Michigan State University, “Nonlocal, Intramolecular Dielectric Functions”
• Jan Jensen, University of Iowa, “The EFP Method: Theory and Biochemical Applications”
• Steven R. Kass, University of Minnesota, “Probing Electrostatic Effects via Experiment and Theory”
• Samuel Krimm, University of Michigan, “Spectroscopically Determined Polarizable Force Fields for Macromolecules”
• Jerzy Leszczynski, Jackson State University, “Molecular Structures and Properties of Complexes with Weakly Interacting Ligands: Shells and Shellvents”
• Nancy Makri, University of Illinois at Urbana-Champaign, “Quantum Dynamics of Large Systems: Recent Developments and Applications”
• Todd Martinez, University of Illinois at Urbana-Champaign, “Generalized Electronegativity and New Models for Charge”
With the exception of the Dirac Award Lecture, which will be announced after the poster deadline, all oral presentation slots are now filled. The plenary presentations, which will take place on Friday morning and afternoon and Saturday morning and early afternoon, will be of equal length and the order of talks will be determined at random.

In addition to the plenary sessions, there will be two poster sessions on Friday evening, October 5. These sessions will showcase the research of graduate students, postdoctoral associates, and senior scientists who are not giving a plenary presentation. A poster mixer featuring pizza and other refreshments will separate the two poster sessions. The deadline for registering to present a poster paper is June 30, 2001.

A number of travel awards are available for poster presenters. Each travel award will be for $200 or actual expenses (transportation, hotel, and other travel related expenses), whichever is less. In addition, the registration fee (which includes the Thursday night, October 4, registration reception, breaks, lunches, and Friday’s pizza poster) is waived for all speakers and poster presenters. Due to the generosity of our industrial co-sponsors, all speakers and at least the first 50 accepted poster presenters (excluding University of Minnesota attendees) will be offered a travel award.

This event is being sponsored by the Supercomputing Institute for Digital Simulation and Advanced Computation, the Army High Performance Computing Research Center, IBM, SGI, Cray, Inc., and Compaq.

Additional conference information will be provided as conference planning progresses. For more information, visit the MTCC’s Internet site:

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Pre-registration is required to attend this conference.
Every second year, the Supercomputing Institute convenes a meeting of its National Advisory Board. Comprised of national experts in several areas of computing, the National Advisory Board meets with Supercomputing Institute researchers and committee members during their visit. The National Advisory Board visited the Institute on November 30, 2000, and was made up of Dr. David Keyes, Lawrence Livermore National Laboratory (front row left), Dr. Albert F. Wagner, chair, Argonne National Laboratory (front row right), Dr. David W. Norcross, Harvard University (back row left), and Professor Robert W. MacCormack, Stanford University (back row right).
Aerospace Engineering and Mechanics

- 2000/221, November 2000
  *Slip Velocity and Lift*
  D. D. Joseph, D. Ocando, P. Y. Huang

- 2001/19, March 2001
  *On an Elastically Induced Splitting Instability*
  P. H. Leo, J. Lowengrub, and Q. Nie

2001/26, March 2001
*Interrogations of Direct Numerical Simulation of Solid-Liquid Flow*
D. D. Joseph

Biochemistry, Molecular Biology, and Biophysics

- 2000/222, November 2000
  *Modeling Passive Mechanical Interaction Between Aqueous Humor and Iris*
  J. J. Heys, V. H. Barocas, and M. J. Taravella

- 2000/225, December 2000
  *3D MHD Simulations of Radio Galaxies Including Nonthermal Electron Transport*
  T. W. Jones, I. L. Tregillis, and D. Ryu

- 2000/226, December 2000
  *Nonthermal Emission in Radio Galaxies from Simulated Relativistic Electron Transport in 3D MHD Flows*
  I. L. Tregillis, T. W. Jones, and D. Ryu

- 2000/232, December 2000
  *Time Evolution of Cosmic-Ray Modified Plane Shocks*
  H. Kang, T. W. Jones, R. J. LeVeque, and K. M. Shyue

- 2000/239, December 2000
  *Cosmic Particle Acceleration: Basic Issues*
  T. W. Jones

Chemical Engineering and Material Science

- 2000/205, October 2000
  *Complex Dynamics within the Vertical Bridgman Crystal Growth Process*
  P. Sonda, A. Yeckel, P. Daoutidis, and J. J. Derby

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• 2000/224, November 2000
   Blade Coating: A Computational Approach to Predict the Experimentally Observed Blade Wear Rate Caused by Particle Impact in Suspension Coatings
   I. Iliopoulos and L. E. Scriven

• 2000/234, December 2000
   Modeling Multiphase Flows Using a Novel 3D Adaptive Remeshing Algorithm
   R. Hooper, V. Cristini, S. Shakya, J. S. Lowengrub, J. J. Derby, and C. W. Macosko

• 2000/238, December 2000
   Modeling the Coupled Effects of Interfacial and Bulk Phenomena During Solution Crystal Growth
   Y. -I. Kwon and J. J. Derby

• 2000/241, December 2000
   Buoyant and Rotational Flows in Small-Scale Vertical Bridgman Growth of Cadmium Zinc Telluride Using Accelerated Crucible Rotation
   A. Yeckel and J. J. Derby

• 2000/242, December 2000
   On Stable Algorithms and Accurate Solutions for Convection-Dominated Mass Transfer in Crystal Growth Modeling
   B. Vartak and J. J. Derby

• 2001/7, February 2001
   Representing Realistic Complexity in Numerical Models of Crystal Growth: Three-Dimensional and Time-Dependent Flows, Phase Boundaries, and Furnaces
   J. J. Derby

• 2000/263, December 2000
   Shape Selective Adsorption in Cylindrical Pores
   S. Mohanty, H. T. Davis, and A. V. McCormick

• 2000/267, December 2000
   Assessing a Flow-Based Finite Element Model for the Sintering of Viscoelastic Particles
   R. Hooper, C. W. Macosko, and J. J. Derby

• 2000/262, December 2000
   Sorbate/Sorbent Phase Transition during Adsorption p-Xylene in Silicalite
   S. Mohanty, H. T. Davis, and A. V. McCormick

Chemistry

• 2000/208, October 2000
   Monte Carlo Calculations for Alcohols and Their Mixtures with Alkanes. Transferable Potentials for Phase Equilibria. 5. United-Atom Description of Primary, Secondary and Tertiary Alcohols
   B. Chen, J. J. Potoff, and J. I. Siepmann

• 2000/209, October 2000
   Monte Carlo Calculations for the Vapor-Liquid Equilibria of Mixtures Containing n-Alkanes, Carbon Dioxide, and Dinitrogen
   J. J. Potoff and J. I. Siepmann

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   Benzocyclobutadienyl Anion: Formation and Energetics of an Antiaromatic Molecule
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   Dodecahedracyl Anion Formation and an Experimental Determination of the Acidity and C–H Bond Dissociation Energy of Dodecahedrane
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RESEARCH REPORTS

• 2000/229, December 2000
  *The Electron as a Protecting Group. 2.*
  Generation of Benzocyclobutadiene Radical Anion in the Gas Phase and an Experimental Determination of the Heat of Formation of Benzocyclobutadiene
  K. M. Broadus and S. R. Kass

• 2000/230, December 2000
  Formation of Gas-Phase Dianions and Distonic Ions as a General Method for the Synthesis of Protected Reactive Intermediates. Energetics of 2,3- and 2,6-Dehydronaphthalene
  D. R. Reed, M. Hare, and S. R. Kass

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**Physiology**

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**Wood and Paper Science**

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