Molecular Science Computing Facility

The Molecular Science Computing Facility (MSCF) supports a wide range of computational activities in environmental molecular research, from benchmark calculations on small molecules to reliable calculations on large molecules, from solids to simulations of large biomolecules, and from reactive chemical transport modeling to regional cloud climate modeling. MSCF provides an integrated production computing environment with links to external facilities and laboratories within the U.S. Department of Energy (DOE) system, collaborating universities, and industry.

Capabilities

Instrumentation & Capabilities

- **MPP2**. Production cluster of 978 HP rx2600 nodes, 1956 1.5-gigahertz IA64 processors, 450-terabytes local disk, 6.8-terabytes memory, and 11.8-teraflops theoretical peak performance
- **Dtemp**. Shared parallel high-performance filesystem on MPP2, 53 terabytes
- **NWfs**. EMSL long-term data store, 300 terabytes
- **Network**. OC12 (600 MBit/sec) internet connection, Gigabit Ethernet MSCF backbone
- **NWVisus**. Visualization server, SGI Onyx 3400Graphics, 8 processors, 8-GB RAM, two Infinite Reality3 pipes, 144-GB disk, with a PanoramTech 3-screen monitor Digital video editing suite
- **Molecular Science Software Suite**. NWChem, Ecce, GA Tools

MSCF provides computational resources for Computational Grand Challenges in environmental molecular science and basic and applied research areas that address the environmental problems and research needs facing DOE and the nation. Computational grand challenge projects typically involve multiple investigators from universities, national laboratories, and industry working collaboratively as teams. These projects are usually granted computer time allocations for three years. MSCF supported 16 three-year grand challenge projects during 2005. The average annual computer time allocation for grand challenge projects in 2005 was 888,324 central processor unit (CPU) hours, an increase of nearly 20 percent over the previous year. This increase is attributed largely to increased stability of the MPP2 computing system.

MSCF also supports smaller, shorter-term projects called MSCF Pilot Projects. Pilot Projects are limited to a maximum of 75,000 processor hours and a one-year duration, with short extensions occasionally granted for project completion. MSCF supported 48 Pilot Projects during 2005, with an average allocation of 49,700 CPU hours. Pilot Projects are typically directed at developing the capability to submit a Computational Grand Challenge proposal in the future (e.g., a combination of theory/method or code development activities, or calculations that provide the initial scientific basis of a Computational Grand Challenge proposal). Pilot Projects are also awarded for computer support of experimental research taking place within other William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) facilities.

A third category of MSCF computer projects are provided to the Office of Science. In 2005 there were 12 such projects allocated for a total of 750,000 CPU hours.

User Computing in MSCF. To optimally address the complex environmental problems facing DOE and the nation and to best use limited staff resources, the EMSL follows the recommendation of the EMSL Science Advisory Committee to use a Computational Grand Challenge approach to providing large blocks of resources to the user community. A call for proposals is issued annually, and teams of computational scientists respond with peer-reviewable proposals for system time allocations. Access for the grand challenge teams is granted for periods of one to three years. The following criteria are used when reviewing proposals:

- scientific merit
- appropriateness of the proposed method or approach
- relevance to the environmental problems and research needs of DOE and the nation
- technical competence of the investigators
- reasonableness and appropriateness of the proposed computer resources.

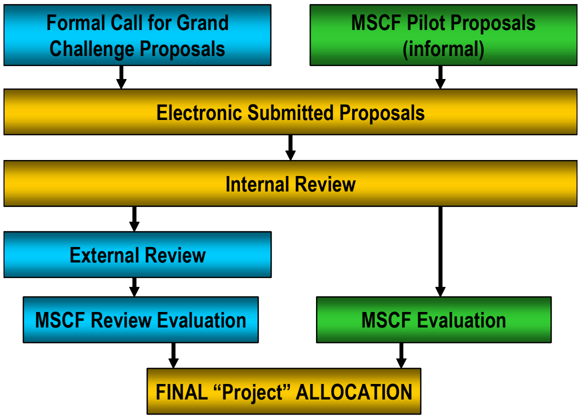

Figure 1. Review process and allocation proposal flow chart.

The process used to review proposals and allocate MSCF computing resources is shown in Figure 1. The request for proposals is open to all researchers, regardless of their institution or source of funding. For reference, the previous request for Computational Grand Challenge proposals involved 22 external scientific reviewers from leading universities and research institutions from around the world. Proposals received two reviews on average, and three reviews in certain cases. A call was not made during 2005 because the computer was over-allocated with current projects; however, a call will be made in 2006.

MSCF Resources

MSCF provides a combination of production computing hardware and software resources and visualization tools to support the scientific research activities of the Computational Grand Challenge and EMSL Pilot Projects. The hardware and visualization resources are the High-Performance Computing System-2 (MPP2), NWfs, the Graphics and Visualization Laboratory (GVL), and the Molecular Science Software Suite (MS^3). These resources are discussed below.

MPP2. MPP2 provides a balanced supercomputer. Since becoming operational in July 2003 with a theoretical peak performance of 1.8 teraflops, 6.8 terabytes of RAM, and 450 terabytes of disk, the Hewlett-Packard supercomputer (Figure 2) has been tailored to meet the operational needs of EMSL users.

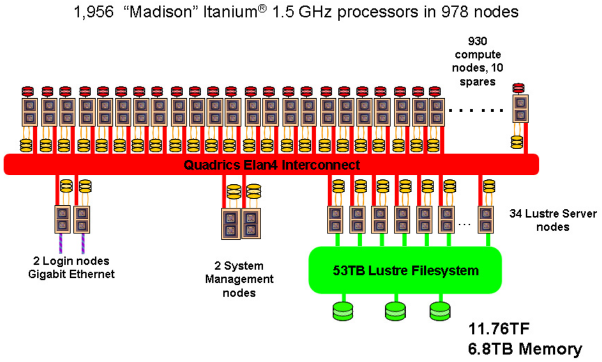

Figure 2. MPP2 Configuration.

NWfs. NWfs, which is the EMSL archive system located in MSCF, uses a groundbreaking approach to disk storage that clusters many low-cost commodity disks to provide fault-tolerant, scalable, long-term storage. Such large-capacity archive systems usually rely on tape for mass storage, but NWfs distinguishes itself by having all its data instantly accessible on disk-based storage. NWfs currently has a capacity of 300 terabytes and the ability to grow as needed to over a petabyte.

GVL. GVL provides production graphics and visualization facilities for the display and analysis of complex datasets from both experiments and simulations. GVL contains four high-performance graphics stations based on Silicon Graphics Incorporated (SGI) technologies with high-speed Gigabit Ethernet connections to the production supercomputers and to NWfs, a digital video system integrated with the workstations to facilitate the display and capture of scientific data, and digital video editing equipment for the preparation of scientific presentations. The video system also is connected to the EMSL auditorium and to the World Wide Web to facilitate internet conferencing. An IBM Scalable Graphics Engine is connected to the MSCF Dell Linux Cluster to provide the highest performance visualization capabilities.

MS^3. Software resources include MS^3, which is a comprehensive, integrated set of tools that enables scientists to understand complex chemical systems at the molecular level. MS^3 couples the power of advanced computational chemistry techniques with existing and rapidly evolving high-performance massively parallel computing systems with extensible problem-solving capabilities. The suite consists of three components: 1) the Northwest Computational Chemistry Software (NWChem), 2) the Extensible Computational Chemistry Environment (Ecce), and 3) the Global Array Tools (GA Tools). These three components are briefly described below.

- ***NWChem***. Version 4.7 of NWChem was released in March 2005. Documentation and information are available on the NWChem Website (http://www.emsl.pnl.gov/docs/nwchem). NWChem provides many methods for computing the properties of molecular and periodic systems using standard Gaussian and planewave-based quantum mechanical descriptions of the electronic wave function or density. In addition, NWChem can perform classical molecular-dynamics and free-energy simulations. These approaches may be combined to perform mixed quantum-mechanics and molecular-mechanics simulations.

  NWChem is available on almost all high-performance computing platforms, workstations, PCs, and clusters of desktop or workgroup servers. NWChem development provides maximum efficiency on massively parallel processors. Among the new features available in the 4.7 version, the following are worth mentioning:
  - A completely new quantum mechanical/molecular modeling module that interfaces between classical molecular mechanics and quantum mechanical modules
  - Several new properties of the density functional theory or Hartree-Fock wavefunctions.

- ***Ecce***. Ecce, which is composed of a suite of client/server Unix-based applications, is a domain-encompassing, problem-solving environment for computational chemistry. Applications for setting up, running, and analyzing the results of computational chemistry studies are built on top of a Web-based data management and inter-application messaging server framework. A computational code registration capability supports several underlying chemistry codes and the ability to integrate new ones without reworking core Ecce applications. Running jobs through industry standard remote communications, like secure shell, and a batch queue management system registration capability allows transparent access to high-performance compute resources from users' desktop workstations. A simple installation procedure and extensive online help combine to make Ecce a preeminent user environment for computational chemistry. The current production release of Ecce is version 3.2.4. There are six major application components:
  1. Calculation Manager aids in the organization and manipulation of computational chemistry studies. This tool allows an at-a-glance overview of the status of every calculation and easy access to key setup parameters and run statistics.
  2. Molecule Builder is an intuitive point-and-click tool that enables the building, visualization, modification, and manipulation of three-dimensional representations of chemical systems.
  3. Basis Set Tool enables users to select from nearly 300 predefined Gaussian basis sets or the ability to create new ones for use in *ab initio* electronic structure calculations.
  4. Calculation Editor allows the user to choose input options using point-and-click interfaces for different chemistry codes, and then generates the code-specific input.
  5. Job Launcher is used for submitting a calculation to a computer for processing. The user may submit a calculation to any computer that has been registered within Ecce and for which the user has an account.
  6. Calculation Viewer provides convenient access to current information for a single calculation during execution or after completion. It has many features for viewing and visualizing chemical system properties.

- ***GA Tools***. GA Tools (also known as ParSoft) includes high-performance computing libraries and tools for applied parallel computing focused on inter-processor communications through the aggregate remote memory copy interface, high-performance input/output through the Parallel I/O tools, and programming models for hierarchical memory systems through the Global Arrays and Memory Allocator libraries. The development of these tools is driven by needs of real scientific application codes on the high-end parallel systems. Development of Aggregate Remote Memory Copy has been supported by EMSL operations and by the DOE Center for Programming Models for Scalable Parallel Computing.

MSCF Organization

MSCF is organized into three project groups: 1) the Visualization and User Services Group, 2) the Molecular Science Software Group, and 3) the Computer Operations Group.

Visualization and User Services Group (VisUS). This group provides an extremely diverse set of services for all users of the MSCF high-performance computers and GVL. Scientists who need access to high-end computing equipment frequently have difficulty getting started. The difficulties encountered range from logging in to getting user codes to run efficiently. VisUS handles user proposal applications, follows user progress during computational projects, manages proposal reviews for both Computational Grand Challenge projects and Pilot Projects, helps with user accounts, provides general consulting support for MSCF software packages, supports and maintains software, manages the GVL, conducts training and user workshops, develops visualization software and high-quality visualizations, and produces Websites.

The group manages the Computational Grand Challenge and Pilot Project proposal process for the MSCF. This activity includes receiving proposals, providing preliminary review for EMSL missions, preparing proposal packets for external peer review, evaluating peer reviews, granting project allocation, and managing the allocations by using GOLD, a dynamic-reservation-based allocations management system originally developed at PNNL.

Consultants have various roles, including those of administrator, tutor, programmer, or research scientist, and field a variety of requests for support. During 2005, five scientific consultants responded to more than 750 e-mail requests, and about 500 additional requests were handled over the telephone or during office visits. Consultants also work directly with MS^3 development teams to give customer feedback and to test functionality.

Information about the use and configuration of the MSCF computational resources is critical to the user base and is provided efficiently to users via the Internet through the MSCF home page. The MSCF Website contains all necessary information about how to establish accounts and get started, and about computer configurations as well as documentation and Web-based tutorials for MS^3. Scientists generate enormous amounts of data either from computational resources or from EMSL instruments. These data are usually complex and difficult to understand. The capabilities and expertise available in the GVL, including its high-performance graphics compute servers and state-of-the-art multimedia equipment, help scientists visualize these complex data. The real-time digital video capture capability from the graphics compute servers allows fast, yet high-quality, video production. Users can generate presentation media in any form—from video (including all international video standards) to Web-based animations. The group also provides basic video production services.

Molecular Science Software Group. This group has the primary responsibility for developing and supporting MS^3. This effort includes:

- developing high-performance versions of the software and new high-performance algorithms
- continually refreshing the underlying software architecture to stay current with new hardware and software technology and standards
- responding to user requests for additional features
- supporting and maintaining the software
- diagnosing MS^3 problems associated with computer vendor hardware and software
- consulting on specific MS^3 problems
- distributing MS^3 to remote sites
- porting software to new architectures
- conducting training and user workshops.

The MS^3 project group focuses on developing next-generation molecular modeling software for newly evolving computer technologies, especially massively parallel computers. The project group is composed of computational chemists and computer scientists (with external collaborations to mathematicians) who work together to develop the MS^3 software. This software is used by many of the MSCF Grand Challenge projects and has been distributed to almost 1200 sites worldwide. In addition to the development activities, this group is also responsible for training software users, conducting tutorial workshops, and providing user support. Several resources have been developed to facilitate user support and training. These resources include MS^3 Websites with user and reference manuals, download information, release notes, FAQs, a list of known bugs, tutorials, and benchmark information, Web-based context-sensitive help available from within the software, as well as a mailing list where users can post support-related questions and get answers either from experienced users or from the NWChem developers.

Computer Operations Group. This group operates, maintains, and advances the capabilities of the MSCF scientific computing systems. The group is responsible for the operation and implementation of the various production supercomputers in the MSCF and has developed unique system management, monitoring, allocation management, and scheduling capabilities. The primary focus is on providing high-quality, reliable production computing cycles and storage capabilities in the MSCF to support very large parallel calculations for Computational Grand Challenge projects.

Upgrades

In 2005 an SGI Tezro Tower VPro 4 processor computer was added to the GLV. This purchase helped replace some of the visualization capabilities lost when one of the 8-processor Onyx 2000 computers became inoperable.

During 2005, NWfs was upgraded from an 85-terabyte collection of discrete NFS servers to a single 300-terabyte Lustre filesystem. The upgrade provided a more reliable and manageable hardware infrastructure, benefiting both MSCF operations staff and users. The transition to Lustre removed constraints on directory sizes, boosted the aggregate transfer rate of the archive, and improved the scalability of the filesystem.

NWChem. Version 4.7 was released in March 2005. In addition to significant performance improvements in several of the existing modules, the following major additions to the capabilities were also delivered:

- A new quantum mechanical/molecular modeling module.
- Properties module expanded with additional nuclear magnetic resonance properties for both self-consistent field (SCF) theory and density functional theory (DFT):
  - Hyperfine coupling (Fermi-Contact and Spin-Dipole expectation values)
  - Indirect spin-spin coupling
  - Shielding now also available for DFT wave functions.
- Task property now requires the specification of the theory (SCF or DFT), making the calculation of properties a single task instead of two (task SCF; task property).
- Ability to use driver for optimization and transition states search for quantum region.
- Self-consistent evaluation of metaGGA energies have been implemented in the DFT module.
- Prototype PBE0 exchange-correlation functional and Hartree-Fock (xc= pbe0, hf) added to PSPW

More information concerning NWChem and the 4.7 release can be found at the NWChem home page, http://www.emsl.pnl.gov/docs/nwchem.

Ecce. Three production releases of Ecce were made in 2005. The first was version 3.2.2 released in February, followed by version 3.2.3 in July, and finally version 3.2.4, which was released in October. Over 430 different sites have downloaded one or more of these three software releases. The total number of unique sites that have downloaded Ecce since version 3.1 was released in August 2003 is more than 750. Featured highlights of version 3.2.2 include:

- support for new Linux operating systems using the GNU C Library version 2.3.2 including Red Hat Fedora Core 3, Red Hat Enterprise Linux Workstation 3, Mandrake 10, SUSE 9, and Debian 3.1
- Ecce download Web page redesigned to simplify choosing the correct distribution for a platform

- users can configure a default number of processors, time and memory limits per machine for running jobs
- Calculation Editor support for the COSMO solvation model built into NWChem
- support for setting up Basis Set Superposition Error calculations through the Builder Geometry Table
- atoms and groups of atoms can be translated directly in the Builder work space by selecting and dragging.

Highlights of Ecce version 3.2.3 include:

- extensive support for the new NWChem 4.7 property runtype including electric fields, electric field gradients, electron densities, shielding tensors, Fermi contact and spin-spin expectation values. Calculation Viewer visualizations include tensors shown as triads of bidirectional vectors and graduated atom displays for scalar data
- support for overlaying visualizations of different properties on top of each other in the Calculation Viewer
- generation and display of hydrogen bonds in the Builder and Calculation Viewer
- support for 64-bit Intel and AMD processors running version 2.3.2 of the GNU C Library
- compression of server-side data enabling up to a 75 percent reduction in disk space usage on the Ecce data server in storing calculation data.

Highlights of Ecce version 3.2.4 include:

- a major update to basis set library data including the addition of new basis sets along with corrections and enhancements to existing ones
- POV-Ray output format enhancements to support hydrogen bond display and anti-aliasing of images for publication quality output
- broader color selection for molecular orbitals in the Calculation Viewer.

In addition to the production releases made in 2005, the Ecce development team has made significant strides in two different areas important to the long-term strategic vision of Ecce. These are end-to-end support for setting up, running, and analyzing results of NWChem molecular-dyanamics simulations and conversion of all Ecce user interfaces to an open-source, cross-platform toolkit. The Ecce 4.0 release in 2006 will be the culmination of the investment in support for molecular dynamics made in 2005. The Ecce 4.0 release will also be the first to feature applications developed with the new wxWidgets cross-platform C++ GUI toolkit. All new molecular-dynamics interfaces are developed with wxWidgets along with a selection of legacy Ecce applications, including the conversion of the Calculation Manager to a new, more robust application named Organizer. The port from the current X Window System Motif toolkit to an open-source, cross-platform toolkit will allow Ecce to run on systems beyond Unix/Linux, including Microsoft Windows and Macintosh OS X. Further, Ecce source code distributions will be possible for the first time, encouraging ports to other hardware platforms by users and contributions of code adding new Ecce capability.

Future Directions

During 2006, MSCF will continue to be a stable production facility focused on accomplishing large, impactful science projects, including support for MSCF Computational Grand Challenges and Pilot Projects, as well as EMSL Grand Challenges, an Office of Science INCITE project, and continuing support and development of the MS^3 software capabilities.

The procurement of the HPCS-3 system will begin in fiscal year 2006, with expected deployment of the system in fiscal year 2007. HPCS-3 will ultimately replace MPP2.

A new petabyte-scale tape library will be procured during fiscal year 2006 and will be deployed to perform backups of MSCF data.

Expansion of the MSCF computer laboratory is scheduled to be completed in September 2006. The 4000-square-foot expansion will double the number of racks that can be accommodated in MSCF and will meet MSCF long-term needs for archive storage space. In the shorter term, the additional space will facilitate the transition from MPP2 to the HPCS-3 system.

MSCF staff will be engaged in many different activities, and through these activities, the staff will continue to build advocacy and awareness of the capabilities available to the scientific user community in the MSCF and EMSL. These activities will include:

- creating information products (e.g., animations of user's research, brochures, fliers, etc.)
- making presentations at national meetings
- organizing symposia in national meetings
- developing tutorials
- establishing an EMSL Distinguished Fellow, associated initially with the MSCF.

Computational Design of Catalysts: The Control of Chemical Transformation

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A catalyst is a substance that speeds up a particular chemical reaction. Catalysts are widely used in chemical industry for the production or processing of materials. Plastics, fuel, and pesticides are just a few examples of materials that are processed, in part, using catalysts. Better catalysts provide the opportunity for quicker and cleaner production of items that we need to live our everyday lives.

Historically, development and discovery of catalysts have been expensive processes of trial and error. For a given reaction type, hundreds or thousands of candidate catalysts must be painstakingly developed and tested before a suitable catalyst is identified. Designing a catalyst from first-principles based on the details of a reaction, a process known as *rational design*, would dramatically impact the field of catalysis because it could help eliminate most of the candidates that are unlikely to succeed, thus providing a substantial reduction in the cost of developing a new catalyst. Rational design has been a long-standing goal of catalysis science, but realizing this vision has remained elusive. However, recent developments in the areas of pure and alloy metal catalysts have the potential to yield catalysts of greatly improved activity and selectivity. Using density functional theory calculations, J Greeley and M Mavrikakis from the University of Wisconsin-Madison discovered a new class of near-surface alloys (NSAs) that can yield superior catalytic behavior for hydrogen-related reactions. Some of these NSAs bind atomic hydrogen as weakly as the noble metals (copper, gold) while, at the same time, dissociating hydrogen much more easily (Figure 1). This unique set of properties may permit these alloys to serve as low-temperature, highly selective catalysts for pharmaceuticals production and as robust fuel-cell anodes. This work represents an important progress in using fundamental first-principles and computational modeling to predict catalysis materials with unique properties. The MPP2 supercomputer, located within the Molecular Science Computing Facility, was partially used to perform these calculations. The results were published as a full paper in *Nature Materials* (Greeley and Mavrikakis 2004) and have been highlighted by the American Chemical Society news magazine *Chemical and Engineering News* (Jacoby 2004).

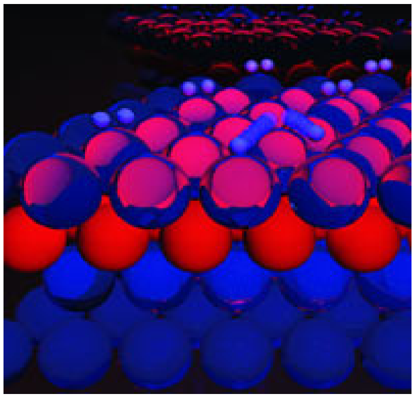

Figure 1. Theoretical studies predict that some alloys consisting of a host metal (large blue spheres) such as platinum or palladium and a subsurface solute (red) such as tantalum or tunsten will make excellent hydrogenation catalysts because of their unique ability to dissociate hydrogen (small spheres) readily and bind atomic hydrogen weakly.

The following publications resulted from this Computational Grand Challenge:

- Greeley J and M Mavrikakis. 2004. "Alloy Catalysts Designed from First Principles." *Nature Materials* 3(11):810-815.
- Harder E, B Kim, RA Friesner, and BJ Berne. 2005. "Efficient Simulation Method for Polarizable Protein Force Fields: Application to the Simulation of BPTI in Liquid Water." *Journal of Chemical Theory and Computation* 1(1):169-180.

Citations

Greeley J and M Mavrikakis. 2004. "Alloy Catalysts Designed from First Principles." *Nature Materials* 3(11):810-815.

Jacoby M. 2004. "Catalysis by the Numbers: Advanced Computational Methods Are Revealing Mechanistic Details and Guiding Catalyst Design." *Chemical & Engineering News* 82(48):25-28.

Accurate Identification of Peptides Using Tandem Mass Spectrometry

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Genes are DNA segments that when "turned on," provide living cells with instructions on how to build proteins. Proteins are molecules, which can be used as the cellular "skeleton," allow some cells to move, process energy and waste products, and participate in virtually every function required for cells to live. Understanding how genes work requires us to obtain a detailed picture of how proteins work.

In recent years, gene sequences have been completed for a wide array of organism types ranging from single-cell bacteria to humans. These genomes are the culmination of worldwide collaborative efforts among academic institutions, private industry, and government agencies. The net result has been the generation of a historically unparalleled amount of publicly available data for organism gene sequences. This information resource continues to grow as the sequences of new organisms are completed. Putting this huge information resource to practical use has brought proteomics, which is the next layer of knowledge, increasingly to the forefront of biology.

Proteomics is the study of proteins in a whole organism under a given set of conditions. Proteins—the molecular "building blocks" in biological systems—perform any number of special functions, allowing cells to live, grow, and react to their surroundings. Proteins are made by joining amino acid residues (smaller molecular units) end-to-end in a particular order that is determined by gene sequence. After proteins reach their final or functional form, they are ready to interact with other proteins, substances inside or outside cells, or genes. Because of their central role in almost all of the processes required to sustain life, understanding protein behavior is a key aspect of understanding any organism's behavior.

To keep pace with the growing demand for proteomic data, high-throughput methodologies have been developed which provide a "snapshot" of all the protein contents of a biological sample. One such method is known as tandem mass spectrometry (MS/MS). Proteins from biological samples being analyzed by MS/MS are first digested with trypsin to produce smaller fragments (peptides), which are then sorted by liquid chromatography elution or some other method. These smaller fragments are then sent to the first stage of the MS/MS process, in which the charge-to-mass ratio of the fragment is determined. In the second phase of MS/MS, the population of identical peptides is broken with high-energy beams, resulting in the collection of small fragments representing the various ways the peptide can be broken. These fragments are sent through a second MS stage, and all of their charge-to-mass ratios are obtained in one dataset. The collection of fragment masses can be thought of as a fingerprint—a profile of peak locations unique for each peptide. Developing methods for accurately identifying peptides from this fingerprint is the aim of Molecular Science Computing Facility (MSCF) Computational Grand Challenge 9603 (Principal Investigator: WR Cannon).

Currently, peptides are identified by creating hypothetical fingerprints of known peptides. The list of known peptides can be any available set of protein sequences and identities. Then for a given spectrum (experimental fingerprint), the similarity to all known peptides of the correct mass-to-charge ratio is calculated, and statistical methods are used to assess the confidence in each similarity score.

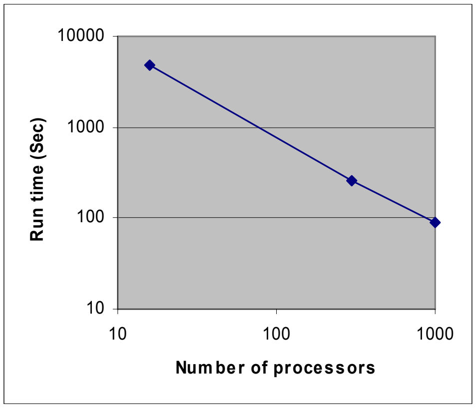

Figure 1. Run time of POLYGRAPH on MPP2.

This peptide identification scheme has been implemented in a software development project, called POLYGRAPH, on two high-performance environments: MPP2, MSCF's 1960-processor Linux cluster, and Altix1, the PACC's 128-processor SGI machine. In both environments, the independent nature of individual spectrum scoring has been exploited to achieve near-perfect speedup. On MPP2, early benchmarks of POLYGRAPH, shown in Figure 1, scaled well to thousands of processors using a protein database with 88,000 entries. Larger databases, such as the non-redundant protein database (nr), may contain millions of entries and must be distributed for POLYGRAPH to function.

Development of the distributed database version of POLYGRAPH has resulted in novel algorithms for managing this massive amount of data in both shared memory and distributed memory architectures. This represents a significant development for capabilities in the growing field of data-intensive computing, and allows for the solution of previously intractable problem sizes using high-performance machines.

The following publication resulted from this Computational Grand Challenge and pilot project:

- Heredia-Langner A, WR Cannon, KD Jarman, and KH Jarman. 2004. "Sequence Optimization as an Alternative to *de novo* Analysis of Tandem Mass Spectrometry Data." *Bioinformatics* 20(14):2296-2304.

Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates

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Fuel cells provide a promising answer to the world's pressing need for clean and efficient power, and play a central role in the "hydrogen-based economy." Investigations of efficient, selective, and less costly electrocatalysts are one of the most active fields in fuel-cell science and technology. This highlight presents interesting results on controlling the catalytic activity of platinum-monolayer electrocatalysts for oxygen reduction with different substrates.

Oxygen reduction at cathodes is a key step for the electrochemistry processes of fuel cells. Extensive attention has been paid to the searching and fine-tuning of electrocatalysts that are highly efficient and selective toward fuel-cell electrode reactions. Currently, platinum metal is widely used as an electrocatalyst for oxygen reduction reactions (ORRs) at fuel-cell cathodes because of its high activity and selectivity toward oxygen reduction. However, platinum is a very expensive noble metal material, and alternatives are needed to reduce the cost for practical application of fuel cells.

Computational and experimental chemists at the University of Wisconsin-Madison and Brookhaven National Laboratory have demonstrated that fuel cells can benefit from coating the cathode with a thin layer of platinum instead of using solid platinum metal. By doing so, the efficiency is raised by 10 percent and the use of expensive platinum can be reduced.

Specifically, electrochemical experiments show that the ORR on platinum monolayers supported on various less-expensive transition metals (e.g., gold, palladium, ruthenium, and iridium) exhibits a volcano-type behavior (see Figure 1). These results are in good agreement with predictions from theoretical calculations performed using plane-wave density functional theory. The calculations also reveal that oxygen-oxygen bond-breaking occurs more easily as oxygen-hydrogen bond-making becomes more difficult, and why the palladium-supported platinum monolayer [Pt_{ML}/Pd(111)] has higher ORR activity than pure Pt(111). These calculations are partially accomplished using the computing capabilities of the Molecular Science Computing Facility.

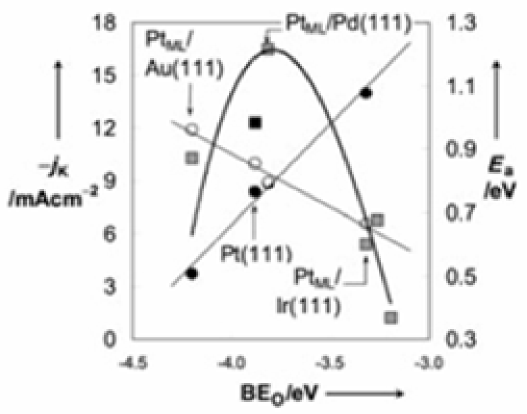

Figure 1. ORR on platinum monolayers exhibits a volcano-type behavior.

The results elucidate, for the first time, that for a good ORR electrocatalyst, the kinetics of both the oxygen-oxygen bond-breaking and the hydrogenation of reactive intermediates have to be facile at the cathode. More importantly and from a practical perspective, it has been shown that it is possible to devise an ORR electrocatalyst that contains only a fractional amount of platinum but can surpass the activity of pure platinum (e.g., platinum monolayer on Pd[111]). Therefore, platinum monolayers supported on appropriate metal substrates represent a viable way to reduce platinum loadings and the associated cost of fuel-cell electrodes. This study, outlined by Zhang and co-workers (2005), also points to the fundamentally important possibility of fine-tuning the electrocatalytic activity of transition metals.

This work was highlighted recently in the chemistry Web magazine *Reactive Reports*.

Citations

Zhang J, MB Vukmirovic, Y Xu, M Mavrikakis, and RR Adzic. 2005. “Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates.” *Angewandte Chemie International Edition* 44(14):2132-2135.

Bradley D. March 2005. “Fuel Cells.” *Reactive Reports*. Number 44, (http://www.reactivereports.com/44/44_1.html).

Reactions of Laser-Ablated Uranium Atoms with Water in Excess Argon: A Matrix Infrared and Relativistic Density Functional Theory Investigation of Uranium Oxyhydrides

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The chemistry of uranium, particularly the hydrolysis reaction, is of major importance in the design of nuclear waste repositories and nuclear fuel reprocessing cycles. Uranium reactions with water have been of great interest because of concerns about the corrosive effect of steam on uranium fuel elements, which is a major safety concern in the operation of nuclear fission reactors. In fact, water is found to act as a catalyst for uranium corrosion in humid air, especially at higher temperatures. This study focuses on the experimental and computational studies of reaction products of laser-ablated uranium atoms with water and a fundamental understanding on the uranium oxo, hydride, and oxyhydride complexes. A series of new uranium species are identified and their structures and vibrational frequencies are assigned.

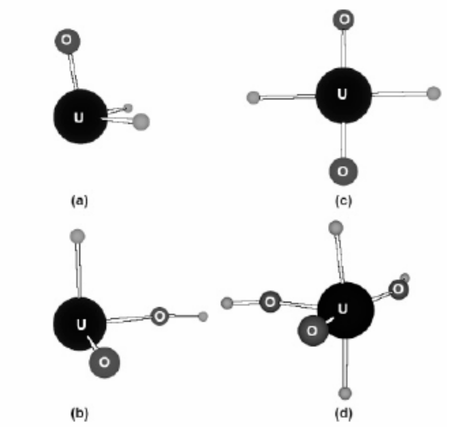

Figure 1. New uranium oxyhydrides, including H_2UO, HUO(OH), H_2UO_2, and $H_2U(OH)_3$ are formed.

In this research (Liang et al. 2005), laser-ablated uranium atoms are used to react with water (H_2O) during condensation in excess argon. A series of interesting new uranium oxyhydrides, including H_2UO, HUO(OH), H_2UO_2, and $H_2U(OH)_3$ (Figure 1), are formed in these reactions. They are identified through infrared spectroscopy and theoretical calculations based on scalar-relativistic density functional theory (DFT). Infrared absorptions at 1416.3, 1377.1, and 859.4 cm^{-1} are assigned to symmetric hydrogen-uranium-hydrogen, antisymmetric hydrogen-uranium-hydrogen, and uranium-oxygen stretching vibrations of the primary reaction product H_2UO. Uranium monoxide, UO, also formed in the reaction, inserts into water to produce HUO(OH), which absorbs at 1370.5, 834.3, and 575.7 cm^{-1}. The HUO(OH) uranium(IV) product undergoes ultraviolet photoisomerization to a more stable H_2UO_2 uranium(VI) molecule, which absorbs at 1406.4 and 885.9 cm^{-1}. Several of these species, particularly H_2UO_2, appear to form weak argon-coordinated complexes based on the calculated uranium-argon distances, binding energies (Figure 2), and the existence of multiple matrix sites, as revealed by the experiments. The predicted vibrational frequencies, relative absorption intensities, and isotopic shifts from relativistic DFT calculations are in good agreement with observed spectra, which further supports the identification of novel uranium oxyhydrides from matrix infrared spectra.

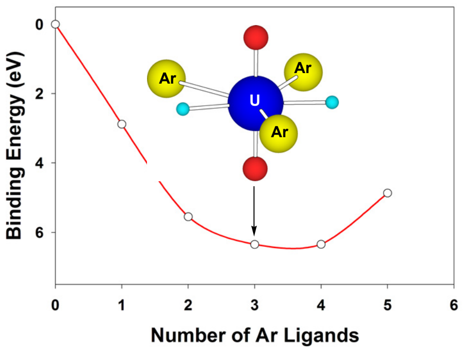

Figure 2. H_2UO_2 appears to form weak argon-coordinated complexes based on the calculated uranium-argon distances, binding energies, and the existence of multiple matrix sites.

The reactions of laser-ablated uranium atoms provide interesting similarities and contrasts to those observed for thorium atoms. For oxidation states of +4 or lower, the chemistry of uranium parallels that of thorium in the formation of species such as H_2AnO and HAn(O)OH. This mutual aspect of thorium and uranium chemistry is largely driven by the high oxophilicity of the early actinide elements. The uranium chemistry progresses into oxidation states higher than can be achieved by thorium, especially in the formation of the U(VI) complexes H_2UO_2 and possibly $H_2UO(OH)_2$. Some of the new molecules reported in this work, especially the U(VI) complexes that have uranium in its highest possible oxidation state, may be involved in the oxidation of uranium in aqueous systems, which is an important issue in nuclear waste remediation.

These calculations were supported through a heavy-element computational chemistry Grand Challenge Project 9598 at EMSL and were performed using the 1960-processor Hewlett-Packard Itanium2 cluster located in the Molecular Science Computing Facility.

Citation

Liang B, RD Hunt, GP Kushto, L Andrews, J Li, and BE Bursten. 2005. "Reactions of Laser-Ablated Uranium Atoms with H_2O in Excess Argon: A Matrix Infrared and Relativistic DFT Investigation of Uranium Oxyhydrides." *Inorganic Chemistry* 44(7):2159-2168.

Multiscale Modeling of Biochip Systems

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Multiscale computational techniques are used to understand the basic physics and chemistry underlying biochip systems. Such systems may be useful for identification of gene mutation, DNA-protein and protein-protein binding, pollutant effects on gene and protein expression, and contaminated water analysis.

Biochip technologies use molecular probes tethered on surfaces for compound analysis. The applications of such technologies are varied and include, but are not limited to, identification of gene mutation, DNA-protein binding, protein-protein binding, pollutant effects on gene and protein expression, and contaminated water analysis. Many of the experimental phenomena observed in these applications occur on time scales that are outside the reach of explicit atom molecular dynamics simulations. This project proposes the use of multiscale computational techniques to understand the basic physics and chemistry underlying biochip systems.

The first part of this project focused on the adsorption of single-stranded DNA on a surface. Single-stranded DNA immobilized on a surface has recently become a popular design for biosensors. The properties of the solid-liquid interface are crucial to both the immobilization of the probe onto the surface and the hybridization of the unknown biomolecule with the target probe. An all-atom molecular dynamics simulation was performed using a 12-base DNA adsorbed onto a 5.1 x 5.3 nm^2 silica surface coated with a layer of positively charged amine groups. Preliminary results reveal that the DNA diffuses to the surface after 40 ns, and, when close to the surface, the DNA adopts a more compacted conformation than the free-solution conformation.

To better understand the dehybridization process by which the duplex unwinds, another molecular dynamics simulation was performed with a duplex DNA strand under melting conditions. Preliminary data show that the ends of the duplex unwind, but total melting does not occur, even after 23 ns. Surprisingly, the system adopts an unusual base-pairing that more closely resembles a Hoogsteen base-pairing for part of the duplex, while the remaining duplex maintains the usual Watson-Crick base-pairings.

Another part of the project focused on protein-DNA complexes. Molecular dynamics simulations of the *Serratia marcescens Endonuclease* monomer with and without DNA were performed. This system exists both as a monomer and a dimer, with both being functional. The results from this simulation revealed that solvent water molecules play an important role. Evaluation of water clusters and pathways in the protein led to the rationalization of a possible mechanism for cleavage of the enzyme.

An investigation into the structural and dynamical solvent properties around hydrophobic solutes was also performed. The mechanism determined for the attractive mean forces between the plates is very different, depending on the nature of the solute-solvent interaction. This has implications for the mechanism of the hydrophobic effect for macromolecules. The focus was shifted to water trapped between the hydrophobic plates, and the results indicated that the translational and re-orientational mobilities of water are much slower at the smaller separation and increases as the separation between solutes becomes larger. This behavior is reminiscent of water behavior in the vicinity of a macromolecule's surface clefts or trapped between two domains of a macromolecule (Figure 1).

The multiprocessor computing facilities in the Molecular Science Computing Facility were used for all calculations presented. Without these facilities, the long-time simulations needed to discern the mechanisms presented would not have been possible.

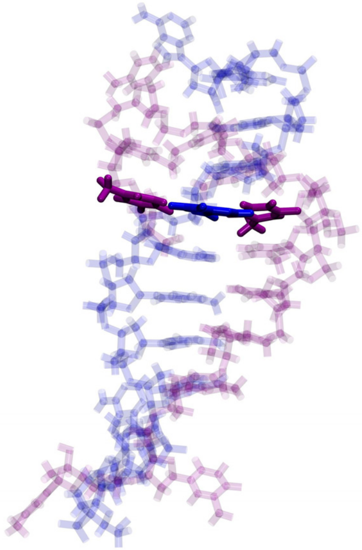

Figure 1. Representation of DNA duplex (translucent) from a snapshot at 10.83 ns. The blue strand is adenine and the red strand is thymine. In the middle region, the thymine (T13) loops back and forms a triplet structure with the adenine (A8, center) and the thymine (T18, right).

Stabilization of Very Rare Tautomers of Uracil by an Excess Electron

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Researchers are studying rare tautomers of nucleic acid bases involved in mispairing of nucleic acid bases in DNA and thus in the development of point mutations. A graphic produced during this research appeared on the cover of the May 21, 2005, issue of Physical Chemistry Chemical Physics.

A tautomer is one of two or more structural isomers—a compound having the same molecular formula but different structures—that exist in equilibrium and are readily converted from one isomeric form to another. Rare tautomers of nucleic acid bases are involved in mispairing of nucleic acid bases in DNA and, thus, in the development of point mutations. PNNL scientists, in collaboration with researchers from the University of Gdansk and Adam Mickiewicz University, are discovering a molecular pathway of destruction of the six-member ring structure of pyrimidine bases by low-energy electrons. In the work described in this highlight, the scientists focused on chemical transformations of nucleic acid bases induced by low-energy electrons. Figure 1 shows a possible mechanism of destruction of the six-member ring structure; this graphic appeared recently in Bachorz et al. 2005.

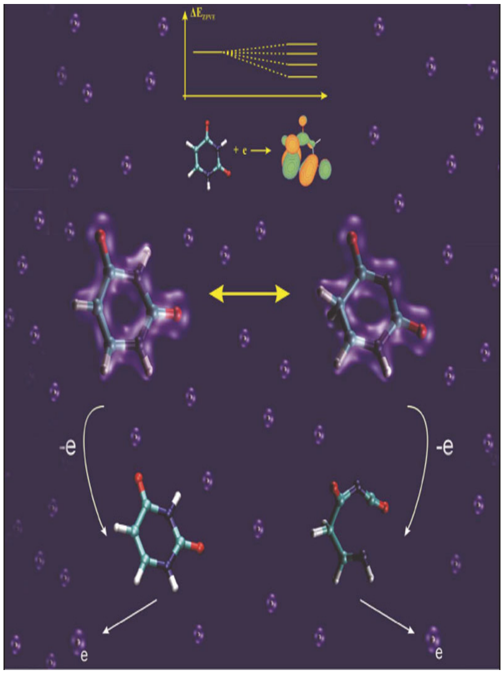

Figure 1. This graphic shows a possible mechanism of destruction of the six-member ring structure of uracil and appeared on the cover of the May 21, 2005, issue of *Physical Chemistry Chemical Physics*.

The principal finding of this research is that low-energy electrons favor very unusual tautomers of nucleic acid bases. These are not canonical or conventional rare tautomers in which proton transfer takes place between electronegative atoms nitrogen or oxygen. Instead, the most stable anionic tautomers result from enamine-imine transformation where a proton is transferred from a nitrogen atom to a carbon atom. These new tautomers might affect the structure and properties of DNA and RNA. In particular, they undergo a barrier-free decomposition of the ring structure of a nucleic acid base upon an excess electron detachment (this is what is shown in Figure 1). These decompositions might be viewed as lesions to DNA or RNA. The new anionic tautomers might contribute to the chemistry of RNA and DNA exposed to low-energy electrons in condensed-phase environments. The investigators will continue to explore this specific area of research.

This research is funded by DOE's Low-Dose Radiation Research Program, which supports fundamental science to determine health risks from exposures to low levels of radiation. DNA damage from radiation-induced mutation is potentially a critical pathway to adverse health effects. For example, single- and double-strand breaks in DNA are induced by lesions formed by low-energy electrons, which are produced in copious amounts by high-energy radiation. The molecular mechanism forming these lesions is not yet known.

Citation

Bachorz RA, J Rak, and MS Gutowski. 2005. "Stabilization of Very Rare Tautomers of Uracil by an Excess Electron." *Physical Chemistry Chemical Physics* (10):2116-2125.

Fast Electron Correlation Methods for Molecular Clusters in the Ground and Excited States

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A new, efficient method allows for highly accurate predictions of large-scale molecular clusters.

The factorial or high-rank polynomial dependence of computational costs with respect to system size is one of the most undesirable features of modern electronic structure theories (Kohn 1995; Head-Gordon 1996). When the system size refers to the volume of a molecule, worse-than-quadratic dependence is argued to be non-physical in view of the two-center nature of Coulomb interactions. The physically correct asymptotic computational cost dependence is, in fact, believed to be linear for extensive quantities (e.g., total energies) and constant for intensive quantities (e.g., excitation energies). By choosing spatially localized functions as a basis set, *fast* electronic structure methods can be devised, the computational cost of which scales in a physically correct fashion (Kutteh et al. 1995; Lee et al. 1996; Strain et al. 1996; White et al. 1996; Challacombe 1999). These fast electronic structure methods have the binary-interaction energy expression of (Kitaura et al. 1999).

$$E = \sum_{i<j}^{n} (E_{ij} - E_i - E_j^{'}) + \sum_{i}^{n} E_{ij}^{'} \qquad (1)$$

Where $E_j^{'}$ is the total Hartree–Fock (HF) energy of unit *i* immersed in the electrostatic field of all the other $n-1$ units and the field is determined, prior to evaluating equation (1), by adjusting the electron density of each unit so that it becomes self-consistent with the field. Likewise, $E_{ij}^{'}$ is the total HF energy of dimer unit *i* and *j* in the electrostatic field created by all the other $n-2$ units. In this project, the researchers combine this binary-interaction method in the dipole approximation with electron-correlation methods ranging from many-body perturbation theory [MBPT(2) and MBPT(3)], coupled-cluster theory [CCSD and CCSD(T)] to density functional theory and with excited-state methods from configuration-interaction singles theory, equation-of-motion coupled-cluster theory (EOM-CCSD) to time-dependent density functional theory. They also consider the inclusion of important three-body Coulomb, exchange, and correlation contributions exactly in what they call the ternary-interaction method. These methods were used to calculate the binding energies of a small water cluster [$(H_2O)_3$], the energy differences among isomers of large water clusters [$(H_2O)_{20}$], the energy difference between the zwitterionic and neutral

Figure 1. The structure of hydrated formaldehyde [$(CH_2O)(H_2O)_{81}$] was calculated using a new approach.

forms of glycine in water [$(C_2NO_2H_5)(H_2O)_7$ and $(C_2NO_2H_5)(H_2O)_8$], the lowest singlet $\Phi^*\leftarrow n$ excitation energies and their solvatochromic shifts of small [$(CH_2O)(H_2O)_2$] and large [$(CH_2O)(H_2O)_{30}$ and $(CH_2O)(H_2O)_{81}$] formaldehyde–water clusters (Figure 1). The largest calculation is performed at the EOM-CCSD level with the aug-cc-pVDZ basis set for a cluster containing 247 atoms.

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Graphene Nanostructures as Tunable Storage Media for Molecular Hydrogen

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Graphene nanostructures can be used as a new media for more effective molecular hydrogen storage.

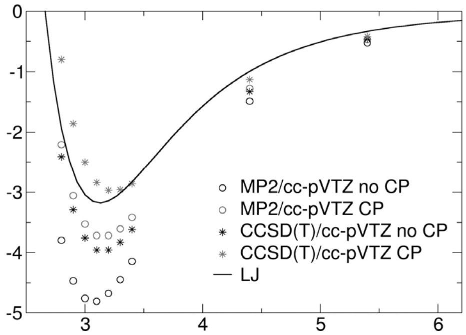

Figure 1. Hydrogen/benzene interaction potentials are calculated using high-level *ab initio* methods.

Many methods have been proposed for efficient storage of molecular hydrogen for fuel cell applications. However, despite intense research efforts, the twin DOE goals of 6.5 percent mass ratio and 62 kg/m^3 volume density (Schlapbach and Zuttel 2001) have not been achieved either experimentally or via theoretical simulations on reversible model systems. Carbon-based materials, such as carbon nanotubes, have always been regarded as the most attractive physisorption substrates for the storage of hydrogen. Theoretical studies on various model graphitic systems, however, failed to reach the elusive goal. Here and in recent work from the *Proceedings of the National Academy of Science* (Patchkovskii et al. 2005), researchers from the National Research Council Canada, and the Technische Universität in Dresden, Germany, show that insufficiently accurate carbon-hydrogen interaction potentials, together with the neglect and incomplete treatment of the quantum effects in previous theoretical investigations, led to misleading conclusions for the absorption capacity. A proper account of the contribution of quantum effects to the free energy and the equilibrium constant for hydrogen adsorption suggest that the U.S. Department of Energy (DOE) specification can be approached in a graphite-based physisorption system. The theoretical prediction can be realized by optimizing the structures of nanographite platelets (graphene), which are lightweight, inexpensive, chemically inert, and environmentally benign. The interaction of nonpolar hydrogen molecules with physisorption substrates in a graphitic system is mainly the London dispersion. Accurate calculations including treatment of electron correlations on model systems, such as polycyclic aromatic hydrocarbons (e.g., benzene and coronene), indicate that hydrogen molecules have adsorption energies between 4 and 7 kJ/mol (Tran et al. 2002; Hübner et al. 2004; Heine et al. 2004) at an equilibrium distance of $a \approx 3$ Å (Figure 2). These binding energies are small and entropic, and quantum effects cannot be ignored at practical temperatures (≈ 200 to 300 K). The estimated limit of accuracy of our calculations at $d \geq 8$ Å is within ±25 percent. Even considering this large margin of error, the researchers conclude that a hydrogen storage enhancement material approaching, or possibly even exceeding, the DOE specification can be produced by encapsulating molecular hydrogen in graphite layers with an appropriate interlayer spacing. All MP2 and CCSD(T) computations were performed with the NWChem program package (Straatsma et al. 2005).

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Quasiperiodic Trajectories in the Unimolecular Dissociation of Ethyl Radicals by Time-Frequency Analysis

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Studies of ethyl radical dissociation processes performed using direct dynamics is helping researchers to understand combustion processes.

The ethyl radical is an important intermediate in hydrocarbon petroleum cracking and combustion processes (Warnatz 1984), playing a central role as the principal precursor to ethylene production through loss of a hydrogen atom. Detailed experimental studies in the relevant high-energy regime had previously worked with the assumption of statistical behavior (Hanning-Lee et al. 1993; Feng et al. 1993). Two recent studies (Gilbert et al. 1999; Amaral et al. 2001) of the dissociation dynamics of ethyl have found that highly excited radicals can dissociate with a fast and slow component, with the slower component decaying four to five orders of magnitude more slowly than predicted by Rice-Ramsperger-Kassel-Marcus theory (Hase et al. 1979), even though the ~5eV excitation energy far exceeds the 1.6-eV barrier to dissociation. Researchers from the Eidgenössische Technische Hochschile in Zürich are investigating the anomalous and unexpected kinetic behavior by means of classical trajectory calculations on a full 21-dimensional, calibrated density functional theory potential surface for C_2H_5. The 410 direct dynamics classical trajectories were integrated with a step size of 0.1 fs for a maximum of 2 ps, or up to a C_2H_4+H center-of-mass distance of 8.0 bohr, whichever came first. The calculations were carried out with a custom version of NWChem (Straatsma et al. 2004). Only 78 percent of the trajectories of ethyl radicals prepared in a microcanonical ensemble with 120-kcal/mol excitation energy above the zero-point energy and zero total angular momentum dissociate to form C_2H_4+H. The remaining hot ground-state ethyl radicals have a lifetime of << 2 ps, during which a time-frequency analysis finds them trapped for extended periods of time in long-lived quasiperiodic trajectories. These calculations support the experimental observation that the dissociation of highly excited ethyl radicals to ethylene and a hydrogen atom can occur much more slowly than predicted by statistical rate theories.

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Are Solvation-Free Energies of Homogeneous Helical Peptides Additive?

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The validities of simple physical models of solvation are tested using free-energy molecular dynamics simulations.

Solvation effects are an important component of many biochemical processes in which solute (e.g. peptide chains) is transferred from an aqueous environment to a less polar medium. The accurate description of solvation effects is therefore an essential part of any systematic approach aiming at contributing to the understanding of such processes.

Methods based on the explicit treatment of solvent using multi-configuration thermodynamic integration (MCTI) or free-energy perturbation approaches provide an accurate and reliable way to calculate solvation effects. This accuracy, however, comes at considerable computational cost, rendering these methods expensive for large systems. Implicit solvent methods represent another way to calculate solvation effects. In these methods, solvent degrees of freedom are not represented explicitly but rather treated as a mean field property. This treatment assumes that solvation-free energy contributions from neighboring segments are to some extent additive. The validity of this assumption is investigated in this work by performing both explicit MCTI and implicit generalized-born surface area (GBSA) model calculations. All MCTI calculations (Figure 1) were performed using the NWChem computational chemistry package. The results of this work indicate that MCTI and GBSA give similar results in the case of five more residues. Sizable differences are found for short peptide chains. Both methods show non-additivity of solvation-free energies for short (less than 5) peptide chains. Other GBSA calculations indicate that additivity is fulfilled for helices longer than 10 residues. These results suggest caution must be exercised when extrapolating implicit solvation parameters from small to large molecules and vice versa.

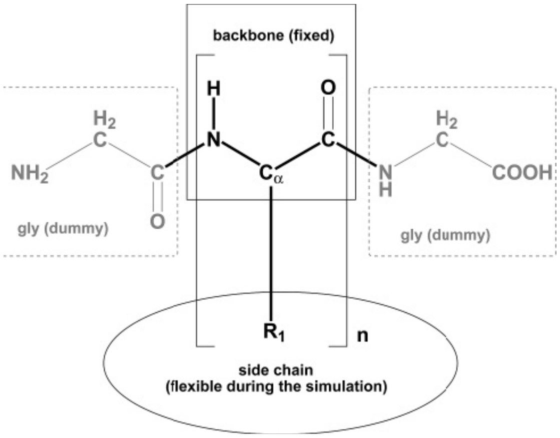

Figure 1. Structure of the system used in molecular dynamics and MCTI simulations.

Analytic Energy Gradients of the Optimized Effective Potential Method

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(a) Duke University, Durham, North Carolina

A new approach to analytical gradient calculations in the optimized effective potential formulation of density functional theory can make complex molecular calculations more efficient.

Analytic energy gradients of the optimized effective potential (OEP) method in density functional theory have been developed. Their implementation in the direct optimization approach (Yang and Wu 2002; Wu and Yang 2003) were carried out and the validity was confirmed by comparison with corresponding gradients calculated via numerical finite difference. These gradients were then used to perform geometry optimizations on a test set of molecules. It was found that exchange-only OEP molecular geometries were very close to the Hartree-Fock results and that the difference between the B3LYP and OEP-B3LYP results was negligible. When energy is expressed in terms of a functional of Kohn-Sham orbitals, or in terms of a Kohn-Sham potential, the OEP becomes the only way to perform density functional calculations, and the present development in the OEP method should play an important role in the applications of orbital or potential functionals.

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Structure and Energetics of Clustered Damaged Sites

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(b) Pacific Northwest National Laboratory, Richland, Washington
(c) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

Computations give insight into damaged and mutated sites in DNA, contributing to a fundamental understanding of radiation effects on DNA.

Quantum calculations on duplex DNA trimers were used to model the changes in structure, hydrogen bonding, stacking properties, and electrostatic potential induced by oxidized purine bases and abasic (AP) sites. Results for oxidized purine bases were consistent with experimental data that show small structural and energetic perturbations induced by isolated 8-oxoguanine (8oG). Watson-Crick base pairing was preserved, and no major distortions of the backbone were induced. The thermal destabilization of DNA induced by 8oG was comparable to the energy of a single hydrogen bond. In contrast, AP sites caused substantial distortions of the DNA backbone that were accompanied by relocation of counterions. The loss of Watson-Crick hydrogen bonds in AP sites had the potential to destabilize DNA by 10 to 20 kcal/mol (0.4 to 0.8 eV); however, new inter- and intrastrand hydrogen bonds formed after removal of a nucleic acid base that significantly affected the energy of AP sites and introduced a strong dependence on sequence context. Quantum calculations on small DNA fragments provided starting conformations and force-field parameters for classical molecular dynamics simulations of radiation-induced, single-strand breaks (Figure 1) that most often combine hydrolysis of a phosphate-oxygen (P-O) bond with an AP site and fully or partially degraded sugar ring. P-O bond hydrolysis increased the freedom in backbone torsion angles, which allowed the broken strand to compress and partially fill the hole in the DNA created by the AP site. Results for strand breaks with a 3'phosphoglycolate were similar to those with phosphate end groups.

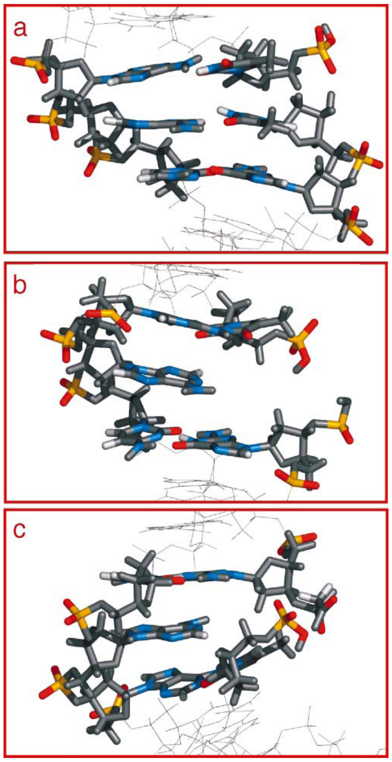

Figure 1. The effect of different types of strand breaks on the conformation of duplex DNA oligonucleotide.

Discovery of "Shrinking New Giant" Mechanism of Fullerene Formation by Quantum-Mechanics/ Molecular-Dynamics Simulations

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Simulations conducted by users of the W.R. Wiley Environmental Molecular Sciences Laboratory from Emory University provide a comprehensive understanding of the formation of carbon nanostructures, with the widest range of promising applications in materials science, molecular electronics, and molecular machinery.

Carbon nanostructures, such as fullerenes (buckyballs) and single- or multi-walled nanotubes, today are the most intensively researched species in the context of molecular engineering on the nanometer scale, with the widest range of promising applications in materials science, molecular electronics, and molecular machinery. Key to the development of highly efficient and commercially viable fullerene generation techniques is the search for the optimal reaction conditions, and development of these techniques requires a comprehensive understanding of the synthesis process.

Researchers at Emory University used the computing resources of the Molecular Science Computing Facility to gain a comprehensive understanding of the formation of carbon nanostructures from a flow of C_2 gas at high temperature (2000 K) and at various high concentrations. They discovered that fullerene formation follows a two-step reaction mechanism. In the first "size-up" step, giant fullerenes with low curvature are readily formed by interaction of polyyne chains, formed from the C_2 molecules, with themselves, which later attached to curved graphene sheets. This process is depicted in Figure 1. In the second "size-down" step, following Smalley's "shrink-wrap" mechanism, giant fullerenes are reduced in size until kinetically stable fullerenes remain. Smaller fullerenes are sometimes formed by losing carbon fragments in "fall-off" or "pop-out" annealing processes under prolonged heating of giant fullerenes. The latter step is found to have a strong dependence on influences such as time and temperature gradient.

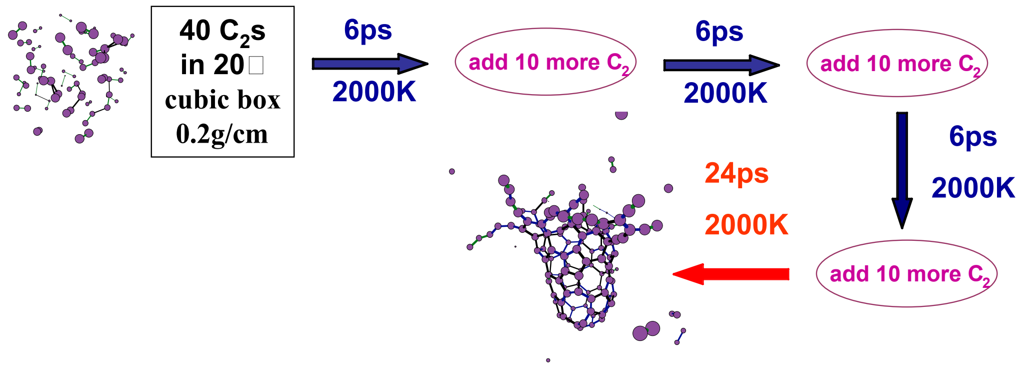

Figure 1. Simulations show that the high-density fullerene formation scheme leads to smaller fullerenes and fewer giant fullerenes.

The combination of subsequent "size-up" followed by "size-down" steps in the formation of fullerenes provides explanations for the appearance of C_{60} and larger fullerenes in combustion and carbon arc experiments and for the existence of readily formed endohedral metal carbide fullerene complexes. The researchers coined the name "shrinking new giant" mechanism of fullerene formation, and suggest that it is universally valid for both carbon plasma as well as polycyclic aromatic hydrocarbon combustion experiments. This research is described in more detail by Zheng and co-workers (2005a, b).

Citations

Zheng G, S Irle, and K Morokuma. 2005a. "Performance of the DFTB Method in Comparison to DFT and Semiempirical Methods for Geometries and Energies of C_{20}-C_{86} Fullerene Isomers." *Chemical Physics Letters* 412(1-3):210-216.

Zheng G, S Irle, and K Morokuma. 2005b. "Towards Formation of Buckminsterfullerene C_{60} in Quantum Chemical Molecular Dynamics." *Journal of Chemical Physics* 122(1):Article No. 014708

Modeling Highly Accurate Energetics of the $(H_2O)_8$ Cluster: NWChem Achieves Over 63 Percent Sustained Efficiency on 1840 Processors

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High-level correlation modeling of water clusters provides researchers with the most accurate interaction energies ever calculated, which will be used to gain insight into water's unique properties. These calculations also demonstrate the unique capabilities of NWChem and the supercomputer, located in the Molecular Science Computing Facility (MSCF) at the W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL).

Researchers from the EMSL and Pacific Northwest National Laboratory used the highly scalable and parallel NWChem software to calculate accurate energetic information of a cluster of eight water molecules. NWChem, the U.S. Department of Energy's premier computational chemistry code, is part of the Molecular Science Software Suite developed at EMSL. The coupled cluster singles doubles with perturbative triples, or CCSD(T), calculation and an aug-cc-pVQZ basis set (1376 basis functions, 32 correlated orbitals) required 1840 processors, almost the entire machine, and 37 hours to complete.

For many years, scientists have attempted to construct simplified descriptions of the intermolecular interactions among water molecules in an effort to gain insight into the unique properties of water from molecular simulations. One bottleneck in this effort is the lack of experimental energetic information regarding the interaction among water molecules that can be used to assess the accuracy of the proposed models. First-principles electronic calculations, such as the calculation described here, offer the advantage of providing this essential energetic information that is the cornerstone in the benchmarking and parameterization of interaction potentials for water.

This huge NWChem CCSD(T) calculation on 1840 processors with a combined peak of 11.04 teraflops sustained an average of more than 63 percent of peak flops efficiency (6.99 teraflops) during the 37-hour calculation, demonstrating the unique capabilities of the NWChem software and the supercomputer architecture. About three-quarters of the time were spent in the triples correction part of the calculation, with a sustained performance of about 84 percent. This part of the calculation consists mainly of some network communication and matrix-matrix multiplication operations, the latter of which is known to achieve more than 90 percent of peak performance on the Intel Itanium-II processor using the Hewlett-Packard Mathematical Software Library. Figure 1 shows a two-hour snapshot of the triples correction part of the performance run.

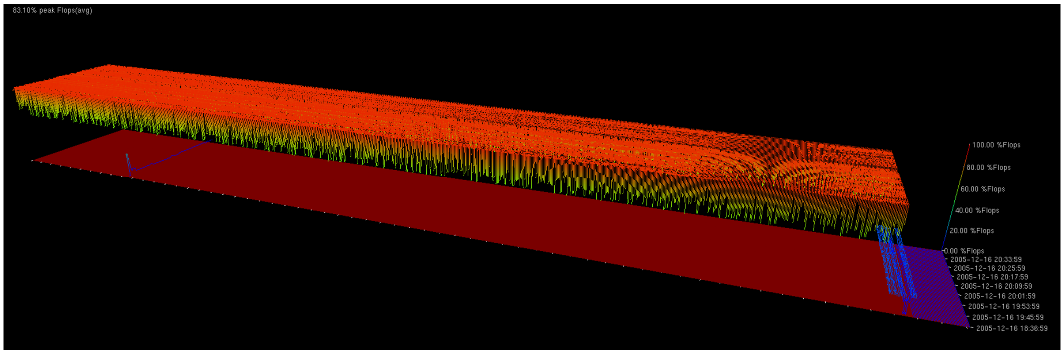

Figure 1. Snapshot of the MSCF system-wide monitoring tool. The vertical axis shows the percentage of peak flops (scale runs from 0 to 100 percent), the axis across the page represents all the processors in the cluster, and the axis perpendicular to the page shows a two-hour window of time slices.

User Projects

Collaborative Development of Software for Electronic Structure Calculations

Council for the Central Laboratory of the Research Councils Daresbury Laboratory, Warrington, United Kingdom
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Calculated Rates of Water-Exchange on Large Aqueous Aluminum Nanoclusters

University of California, Davis, Davis, California
AG Stack, WH Casey

Coupled Quantum Simulation Techniques for Studying Nanostructured Materials

Lawrence Livermore National Laboratory, Livermore, California
AJ Williamson, F Gygi

Correlation of Structure and Function of Zinc Metalloproteins via Solid-State Nuclear Magnetic Resonance (NMR) Methods

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Fast-OS PetaScale Linux

Oak Ridge National Laboratory, Oak Ridge, Tennessee
RS Studham

Single-Enzyme Nanoparticle Crosslinking Polymerzation

Pacific Northwest National Laboratory, Richland, Washington
MC Perkins

Sub-Grid Modeling of Diesel Particulate Filtration Using the Lattice-Boltzmann Method

Pacific Northwest National Laboratory, Richland, Washington
ML Stewart

Computer Simulation of Optical Spectroscopy

Pacific Northwest National Laboratory, Richland, Washington
H Lu, D Pan

Molecular Modeling

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Integrated Multiscale Modeling of Molecular Computing Devices

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Oak Ridge National Laboratory, Oak Ridge, Tennessee
RJ Harrison

Animation for Morphing Catalysis

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MC Perkins

MP2/CBS Pair Corrrelation Function of Liquid Water

University of Delaware, Newark, Delaware
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High-Performance Computing Challenge Benchmark

W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington
KM Fox

Simulation of High-Voltage, Direct-Current Converter Valve Control and Protection Algorithms

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JM Johnson

Quantification of the Ligand Effects in Transition Metal Coordination Compounds Using Electronic Structure Calculation Methods

Aristotle University of Thessaloniki, Thessaloniki, Greece
CA Tsipis, C Kefalidis

Establishing Benchmarks for Stability Testing of Future Intermediate Range Compute Server

Pacific Northwest National Laboratory, Richland, Washington
LR Corrales, V Glezakou

Fluorescent Labeling of Proteins Based on Known Crystal Structures

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First-Principles Catalyst Design for Environmentally Benign Energy Production

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Comparative Molecular Trajectory Analysis

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Real-Time Atomistic Simulation Studies of Light Harvesting and Charge Transport for Hydrogen Production in Solar Cells

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Comparative Protein Structure Modeling: From Protein Sequence to High-Accuracy Protein Structure

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High-Fidelity Direct Numerical Simulations of Turbulent Combustion: Compression Ignition under HCCI Conditions and NOx for Turbulent Jet Flames

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Wet Electrons at Metal Oxide Surfaces

University of Pittsburgh, Pittsburgh, Pennsylvania
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Snow Pack Predictions for the Next 50 Years in the Pacific Northwest

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MC Perkins

Molecular Modeling of Electron Transfer in Fe(III) Oxides

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Megaports Training Video Development

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Joint Application of Theory and Experiment to the Chemistry of Environmentally Important Organic Peroxides

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High-Performance Sequence Analysis for Data-Intensive Bioinformatics

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Proton Transport in Polymer Electrolyte Membranes

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De Novo Structure-Based Molecular Design

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Comparison of Thermal Signature of Air-Cooled RX2600 Node with SprayCool FX2600 Node

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Immobilization of Radionuclides in Oxides

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Development of GASNet Communication System on the Quadrics Interconnect

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A Computational Approach to Understanding Aerosol Formation and Oxidant Chemistry in the Troposphere

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Biomolecular Simulation of Base Excision Repair and Protein Signaling

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Effects of the Presence of Helium on Silicon Carbide

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Chemical Fate of Contaminants in the Environment: Chlorinated Hydrocarbons in the Groundwater

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Geometry Optimizations of Aqueous Aluminum Clusters

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Determining the Phase Behavior of Polarizable Water Models

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New Approach to Extract and Visualize Discontinuities from Two-Dimensional and Three-Dimensional Seismic and Imagery Datasets

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Intrusion-Detection Video

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Computational Fluid Dynamics Applied to Airflow Problems in Animal and Human Lungs

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Ab Initio Calculations of Guanosine Triphosphate (GTP) Hydrolysis by Using NWChem and TAO Components

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Local Motions in Protein Structures

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Electronic Structure Calculations of Hydrogen Bonding in Biological Macromolecules

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AV Morozov Benchmarking Climate and Weather Modeling Codes on the Pacific Northwest National Laboratory (PNNL) Cluster

Hewlett-Packard Company, Richardson, Texas
L Sankaran

Computer Simulation of Radiation Effects in Zircon

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A Grid-Based Exact or High-Accuracy Solution of the Electronic Schrödinger Equation

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Complex Enzymatic Reactions Studied by Molecular Modeling and Electronic Structure Calculations

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Benchmarking Localized Coupled Cluster methods in the NWChem Package

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Modeling Dynamically and Spatially Complex Materials

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Modeling Complex Bacterial Cell Systems Through Development of Segregated Models with Spatial Localization

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Superparameterization: A New Paradigm for Climate Modeling

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Molecular Computational Studies in Environmental Chemistry, Geochemistry, and Biogeochemistry

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Computational Study of Protein-Protein Interaction Dynamics

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Multiscale Modeling of Biochip Systems

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Nanostructure Formation, Aggregation, and Reactivity

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Multifluid Flow and Multicomponent Reactive Transport in Heterogeneous Subsurface Systems

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Molecular Energetics of Clustered Damage Sites in DNA

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Direct Dynamics Simulations: From Molecules to Macromolecules and Condensed Phases

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Accurate *Ab Initio* Determinations of Thermochemical Properties of Environmental and Biological Molecular Systems for Benchmark with Experiments

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Nuclear Magnetic Resonance (NMR) Chemical Shift Calculations for Novel Bioactive Metabolites from an Acid Mine Waste Organism

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Image Processing, Modeling, and Simulation of Complex Biological Systems

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Computational Fluid Dynamics (CFD) Code Performance Testing

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Computed Frequencies to Support Experimental Quests for Novel Molecules

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Common Architecture Chemistry Components for Terascale Simulations

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Rosetta *Ab Initio* Protein Folding

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Computational Characterization of Two Lesions in DNA: 8-Oxo-Adenine and Abasic Site

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A New Approach to Protein Folding by Reducing Dimensionality of Protein Conformational Space

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Animation and Three-Dimensional Illustrations for the Atmospheric Radiation Measurement Program

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Multi-Region Reactive Transport due to Strong Anisotropy in Unsaturated Soils with Evolving Scales of Heterogeneity

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Epidermal Growth Factor Receptor (EGFR) Dimerization

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Deploy Lustre as a Global Filesystem on the HPCS2 Supercomputer

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Pacific Northwest National Laboratory (PNNL) Facilities Master Plan

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Ab-Initio Simulations of the Catalytic Mechanism in Protein Kinases

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Fundamental Assessment of the Accuracy of Time-Dependent Density Functional Theory

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Radiation-Detection Portals for Border Security

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Defects, Defect Processes, and Ion-Solid Interactions in Ceramics

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Computational Chemical and Materials Science to Study Nanoscale Surface Reactivity and Radiation Resistance of Metal Oxides

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Direct Numerical Simulations of Turbulent Combustion: Temperature Inhomogeneity Effects on the Autoignition of Hydrogen/Air Mixture Spontaneous Ignition Regime

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Quantum and Classical Simulations of Clusters, Self-Assembly, Nano-Scale Manipulations, Nanotribology, and Biological Processes

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A Combined Approach for Protein Structure Prediction

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Multimedia for Investigator Training

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Aerosol Model Data Storage

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Investigating Three-Dimensional Coupled Geophysical Processes of the Subsurface

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Oxidation and Radiation Damage in Nucleic Acid Bases

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Electronic Structure Study of Platinum Clusters

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NAMD Benchmarking on W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) Molecular Science Computing Facility for Molecular Dynamics Simulations

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Chemical Discovery Through Advanced Computing

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Energetics, Bonding Mechanism, and Electronic Structure of Metal/Ceramic Interfaces

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Physical Chemistry of Heterogeneous Processes

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Pacific Northwest National Laboratory (PNNL) Next-Generation Chemistry-Meteorology-Aerosol Model

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Ab Initio Calculations on a Proposed Gating Mechanism for the KcsA Channel

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Modeling Dynamically and Spatially Complex Materials

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Studies of Long-Time-Scale Processes of Environmental Importance

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Immune Response to Environmental Factors: Molecular Dynamic Simulations of Antibody Structure

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Computational Design of Materials for Hydrogen Storage

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Reliable Relativistic Quantum Chemistry Calculations for Molecules with Heavy Elements

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Computational Design of Catalysts: The Control of Chemical Transformation

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