



Jefferson  
Lab's  
Xiaochao  
Zheng

## Research Highlights . . .

*DOE Pulse* highlights work being done at the **Department of Energy's** national laboratories. **DOE's laboratories** house world-class facilities where more than 30,000 scientists and engineers perform cutting-edge research spanning DOE's science, energy, national security and environmental quality missions. *DOE Pulse* ([www.ornl.gov/news/pulse/](http://www.ornl.gov/news/pulse/)) is distributed every two weeks. For more information, please contact Jeff Sherwood ([jeff.sherwood@hq.doe.gov](mailto:jeff.sherwood@hq.doe.gov), 202-586-5806).



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### ADVISOR: Proper pressure saves fuel

Engineers at DOE's **National Renewable Energy Laboratory** recently completed a series of simulations for **ADVISOR**, a hybrid electric vehicle simulation model, to be included in the California Energy Commission's report on fuel-efficient tires. The simulations used the new **ADVISOR** rolling resistance model to show the impact of rolling resistance and tire pressure for the fuel economy of a Ford Focus. Results show that purchasing low rolling resistance tires and maintaining proper tire pressure can provide significant fuel savings. The results are being included in a report to the California legislature as part of Senate Bill 1170 on energy resource conservation.

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### Clarifying Real Compton Scattering

Physicists at DOE's **Jefferson Lab** are busy analyzing data from their Real Compton Scattering experiment, which explores the scattering of low-energy photons off the proton at large scattering angles—where the quark structure of the proton is expected to be revealed best. The experiment tests whether, during scattering events, a photon bounces off a quark in the way described by Arthur H. Compton for scattering from isolated electrons, and as predicted by a JLab theorist. Or does the scattering involve the cooperative behavior of three quarks, as predicted by perturbative Quantum Chromodynamics? Preliminary results indicate that protons are polarized along their line of momentum, confirming the single-quark scattering mechanism advocated by JLab scientists.

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### SLAC, Fermilab collaborate on linac structure

In late 2002 a two-foot long linear particle accelerator section from **Fermilab** arrived at DOE's **Stanford Linear Accelerator Center**. It is one of the first fruits of the collaboration between these two high-energy physics labs working to design and build a proposed new collider. Their collaboration is focused on learning to build accelerator sections in a manner consistent with efficient industrial methods. The new collider would need tens of thousands of these structures, so it would be necessary to contract them out to industrial manufacturers for fabrication. The Fermilab structure, and the dozen that will follow, will function as a test and demonstration of the basic linac accelerator system unit and of the international collaboration.

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### Hardware enhances long-distance collaborations

Near-real time **interactive remote-visualization hardware** that enables people separated by thousands of miles to share and collaborate on information has been developed at DOE's **Sandia National Laboratories**. Research team leader Lyndon Pierson says the technology is expected to be of interest to oil companies, universities, the military, medicine—"anywhere people have huge quantities of visualization data to transmit and be jointly studied." The hardware leverages advances in 3D commercial rendering technology and compresses the video data flooding in at nearly 2.5 gigabits a second into a network pipe that carries less than 0.5 gigabits a second. It was demonstrated successfully in late October between Chicago and Amsterdam.

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# It's all in the GAMESS

Scientists at DOE's [Ames Laboratory](#), led by Mark Gordon, director of the Lab's Applied Mathematics and Computational Sciences Program, are fostering and expanding a computational chemistry code that provides extensive and detailed information about how things work on the molecular scale. The General Atomic and Molecular Electronic Structure System, or GAMESS, includes a hierarchy of quantum chemistry methods that helps solve problems relating to molecules. Using GAMESS, the



**Mark Gordon, head of Ames Laboratory's Scalable Computing Lab, visits with Secretary Abraham about GAMESS and other SCL efforts that take advantage of parallel power at SC2002 in November.**

Gordon group is making major contributions to the design of new rocket fuels for the Air Force and new optical materials, fuels and wear-resistant coatings for the Department of Defense.

GAMESS is a "legacy" code that was assembled in 1977 from existing quantum chemistry computer programs by the staff at the National Resource for Computations in Chemistry. The project ended in 1981, but the Gordon group has continued to enhance the software suite over the years, developing new functionalities and parallelizing the code.

The researchers have created sophisticated and complex methods for GAMESS to address intermediates, unusual chemical species that may have lifetimes of only picoseconds or femtoseconds, but may be very important in the overall chemical reaction.

In addition, GAMESS includes the novel graphics visualization programs, MacMolPlt and WinMolPlt, for Macintosh computers and PCs, respectively. The programs ease the task of interpreting the complicated calculations performed by GAMESS.

A unique feature of GAMESS is the effective fragment potential, or EFP, which is based on quantum mechanics but is not quantum mechanics. The EFP is a sophisticated model to predict how solvents effect chemical reactions and to predict the behavior of liquids. Treating a molecular system with EFPs makes it possible to complete an entire calculation in orders of magnitude less computer time than a fully quantum calculation. GAMESS is distributed at no cost to users by accessing [www.msg.ameslab.gov](http://www.msg.ameslab.gov) and signing a license agreement.

*Submitted by DOE's [Ames Laboratory](#)*

## DETERMINED YOUNG WOMAN ENTERS WORLD OF SUB-NUCLEAR PHYSICS



**Xiaochao Zheng** then switched to physics for her master's because she wanted more of a challenge.

In China, completing middle and high school usually takes six years, but Xiaochao Zheng finished a gifted program in just four years; and at 14 entered a prestigious university. She earned a bachelor's degree in engineering in 1996; She was accepted at the [Massachusetts Institute of Technology](#) in 1999. During her second semester she undertook the analysis of results from a Helium-4 experiment conducted at Mainz, Germany. Within six months she learned about a host of experimental details, and brought the data analysis to the 90% completion point for publication, all while taking a full load of graduate courses.

After only a year of classes she passed the written parts of the doctoral qualification exam with flying colors, and set about starting research for her thesis. She headed for DOE's [Jefferson Lab](#) in June 2000 and quickly established herself as a determined and effective student. She took on many night shifts on experiment data runs to master the equipment she would use in her research, which involved deeply inelastic scattering of polarized electrons from polarized Helium-3. She familiarized herself with all aspects of the experiment, tested and improved the target system, and made valuable improvements to the laser and optics and electron paramagnetic resonance polarimeter systems. During the four month experiment run, Xiaochao played a key role in ensuring data quality and in diagnosing experimental problems.

She completed her doctoral program in December 2002—a breathtaking 3-1/4 years—and has accepted a post-doctoral position at DOE's Argonne National Lab.

When asked about herself, Xiaochao said, "I'm just a plain and shy person, but I would like to share the following saying I try to follow: "Dream is not in the sky but in your heart. Success is not on the ground but under your feet."

*Submitted by DOE's [Jefferson Lab](#)*