



LLNL's Dona Crawford

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## Research Highlights . . .



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### An exceptionally effective lead-detection protein

Scientists from DOE's [Brookhaven National Laboratory](#) and the [University of Chicago](#) have discovered that a member of a well-known protein family is better at detecting lead than any other known substance. In fact, the protein is more than one thousand times more likely to bind to lead than other metals, such as mercury, zinc, or copper. Learning more about the protein's structure and lead-detection mechanism may lead to new ways to synthesize drugs or to develop treatments for lead poisoning, a worldwide problem that, in the U.S. alone, inflicts irreversible physical damage to half a million children each year.

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### DZero sets new top for top quark measurement

The [DZero collider experiment](#) at the Department of Energy's [Fermilab](#) has completed two preliminary measurements of the top quark mass using data from [Run II of the Tevatron](#). The result—170.6 +/- 7.3 GeV/c<sup>2</sup>—is the most precise measurement of the top quark mass from Run II data to date. The Tevatron, where the top quark was discovered in 1995 by the DZero and [CDF experiments](#), is still the only source of top quarks. Measuring the properties of the top quark in detail makes it possible to test theoretical predictions, such as the connections between the top, the W boson and predictions for the mass of a Higgs boson.

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### New system fights corrosion

Researchers at DOE's [Pacific Northwest National Laboratory](#) have made a key advance in developing a fully automated system that fights corrosion and wear and tear in even the hardest-to-reach places. The [Electrospark Deposition, or ESD](#), system is a fully automated apparatus that transfers a very low heat, controlled weld of a metallic coating onto surfaces that may become corroded. A computer monitors the spark current, which indicates the contact force, and adjusts the equipment to maintain the optimum contact force. Users of the system can align the part, start the computer, and return when the application is completed. It can be particularly useful in industries where large quantities of repairs are needed, such as aviation and aerospace, military hardware, medical, timber, automotive and food processing. PNNL recently licensed the ESD automation technology to Advanced Surfaces and Process Inc. of Cornelius, Oregon.

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### Chemical guidebook may help Mars rover track extraterrestrial life

To help a NASA rover eventually hunt for life on Mars, [Idaho National Laboratory](#) scientists are writing a chemical guidebook to aid the search for extraterrestrial life. Using new imaging tools and earthly parallels of ancient Mars environments, they're recording the types of subtle chemical changes that Martian microbes may have left on the planet's rocks. The researchers hope someday to arm a Mars rover with a suite of tools – a guidebook, precise chemical imagers, and human-like reasoning ability – and let it search for signs of alien life on its own.

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# NETL, university advance hydrogen production research

**D**OE's national laboratory system encourages collaborative efforts with universities and private industry to address the nation's energy and environmental problems.

Researchers at DOE's [National Energy Technology Laboratory](#) and [Carnegie Mellon University \(CMU\)](#) of [Pittsburgh, Pa.](#), have longstanding experience in conducting research and applying computational modeling to energy-related problems. They are collaborating to combine computational and experimental methods to test a variety of hydrogen separation membranes that seem to have the potential to remove hydrogen from mixed gas streams and simultaneously remove impurities from the hydrogen product. Although hydrogen is very abundant, producing it from fossil fuels, water, or renewable energy sources is very costly. With a goal of reducing the cost of hydrogen production, researchers at NETL and CMU are studying hydrogen gas separation.



*PdCu Membrane*

Selecting the most cost-effective membranes to separate hydrogen from mixed gas streams through laboratory experimentation is both time-consuming and expensive. NETL and CMU researchers have been collaborating to develop better methods to determine the optimum composition of membranes. Coupling the predictive capability of

computers with laboratory experiments, the researchers were able to develop a computational method for screening alloys using theoretical models.

By screening candidate alloys with special computer programs to determine the ones with the best separation potential, researchers save time and money by avoiding the need to create a multitude of alloys and then test their properties in a laboratory setting. Using computational chemistry, only the most promising alloys would be subjected to experimentation.

NETL researchers have demonstrated recent successes with a new hydrogen membrane material made of palladium and copper (Pd-Cu) alloy. Their results to date have shown the ability of the membrane—resembling a flat disc about three-fourths inch in diameter\* to allow pure hydrogen to pass through without contamination of the membrane by other gas impurities (such as hydrogen sulfide) during the separation process.

The team's research, supported by DOE's Office of Fossil Energy, appeared in the January 28, 2005, issue of the prestigious journal *Science* published by the American Association for the Advancement of Science.

*Submitted by DOE's [National Energy Technology Laboratory](#)*

## LLNL's DONA CRAWFORD SETS BLUEGENE'S PACE

Dona Crawford, the Associate Director of [Lawrence Livermore National Laboratory's](#) Computation Directorate, is responsible for the development and deployment of integrated computing and information environments capable of terascale simulations.



*Dona Crawford*

"These machines are the backbone of science and technology," Crawford said. "The simulations performed on these machines will enable virtually every scientific field for decades to come."

Crawford, was recently named to the Alameda County Women's Hall of Fame in the Science category for her work and her leadership in establishing the world fastest supercomputer, called Blue Gene/L, at Lawrence Livermore.

"I am honored to accept this award on behalf of the large team of scientists and engineers at the Lab, at IBM (BlueGene/L's developer) and at DOE/NSA who made it possible," Crawford said. "It's even more rewarding because of its significance and importance to the Laboratory and its missions."

Last November, Blue Gene/L took center stage in the technological world when the supercomputing industry proclaimed the computer the world's fastest computer on the [Top500 list](#). At 70.72 teraflops, or trillion operations per second, Blue Gene/L outpaced the previous top performer, Japan's Earth Simulator, which had held the top spot for three years. Blue Gene/L was just one quarter of its eventual capability; since that time the second quarter of the machine has been installed and [has achieved 135.3 teraflops](#).

Blue/Gene L will be used to ensure the safety and security of the nuclear stockpile and set the stage for myriad breakthroughs in chemistry, physics, engineering, medicine and materials science.

She also promotes math and science careers for young women in the Tri-Valley area through her participation in community outreach activities such as the Expanding Your Horizons conferences held three times each year, the Go Figure Math Competition and numerous high school achievement awards.

*Submitted by DOE's [Lawrence Livermore National Laboratory](#)*