

LIVERMORE LAB REPORT

A weekly review of scientific and technological achievements from Lawrence Livermore National Laboratory, Jan. 30-Feb. 3, 2012



RESHUFFLING THE DECK



The Sequoia supercomputer

Though China and Japan most recently have nabbed the top five spots on the list of the Top 500 supercomputers, a reshuffling is imminent.

This year, America is limbering up for a comeback. Three of its national labs are being spruced up and Lawrence Livermore will be high up on that list once again.

The first racks of a 20-petaflop BlueGene machine, Sequoia, have already been delivered to the Lab, and the machine is expected to go online later this year. (Computing power is measured in so-called floating-point operations per second, or flops; a petaflop is a million billion flops.)

This month, the Department of Energy will set out its plans to broach the so-called exascale by the end of the decade. One goal is an exaflop computer, which would use less than 20 megawatts of power.

To read more, go to [The Economist](#).



The planet GJ 1214b, shown here in an artist's conception with two hypothetical moons, orbits a "red dwarf" star 40 light years away from Earth. *Image credit: Center for Astrophysics/David Aguilar*

Using models similar to those used in weapons research, scientists may soon know more about exoplanets, those objects beyond the realm of our solar system.

In a new study, Laboratory scientists and collaborators came up with new methods for deriving and testing the equation of state (EOS) of matter in exoplanets and figured out the mass-radius and mass-pressure relations for materials relevant to planetary interiors.

Astronomers started detecting exoplanets 18 years ago and more than 700 have been found so far, the vast majority within the last two years. Interest is now growing in the structure and atmospheres of these worlds.

To read more, go to [R&D](#).



Navajo Nation President Ben Shelly (left) and Laboratory Executive Officer Ron Cochran sign the Memorandum of Understanding that will further mutual energy collaborations between LLNL and the Navajo Nation.

The Laboratory and the Navajo Nation signed a Memorandum of Understanding (MOU) this week to further mutual energy collaborations.

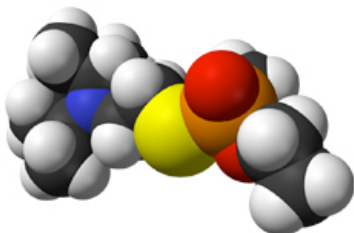
LLNL and the Navajo Nation plan to collaborate in an array of areas including energy security; carbon sequestration; coal gasification; shale gas; enhanced oil recovery; wind, geothermal and solar; environmental studies and other areas.

The MOU comes on the heels of newly developed policy for the Navajo Nation -- one that intends to protect the energy, natural resources and assets of the nation, create a self-sustaining economic future, and supply Navajo communities with the benefits afforded by energy development through total resource sovereignty.

To read more, go to the [Associated Press](#).

Chemistry World

A SAFER PATHWAY



A 3D model of the chemical agent VX.

Computers can make finding new ways of decontaminating the deadliest known chemicals safer and easier.

VX, made infamous by the 1996 Nicolas Cage film "The Rock," is the most toxic nerve agent known and also is highly persistent. Although banned by the Chemical Weapons Convention, it is still important to understand and find new decontamination pathways to counter the threat of terrorism.

Richard Gee and his Laboratory team have shown that using first principles molecular dynamics (FPMD) can reduce the number of dangerous experiments needed. They used their FPMD model to simulate known oxidation and hydrolysis pathways and compared their results to experimental findings. They were able to validate their method for understanding how VX interacts with decontamination solutions, thereby reducing the number of necessary experiments.

Although there have been other theoretical studies on VX decontamination, the researchers stress that this is the first time the solvent has been treated explicitly, allowing for a much more accurate simulation.

To read more, go to [Chemistry World](#).



STREAMING SCIENCE

The Laboratory's popular lecture series, "Science on Saturday," returns this Saturday (Feb. 4) and runs through March 3. This year, attendees also will be able to watch the talks, which will be streamed live, from any computer.

The lectures are free of charge and will be held in the Bankhead Theater, located at 2400 First St. in Livermore. Two presentations are offered at 9:30 a.m. and 11:15 a.m. This year, the Lab is expanding the availability of the talks by streaming them live via the [LLNL Facebook page](#).

This year's talks cover a wide range of current topics including the Lab's work on the Mercury Messenger; effects of earthquakes; space junk; and restoring sight to the blind.

To read more, go to the [Web](#).

LLNL applies and advances science and technology to help ensure national security and global stability. Through multi-disciplinary research and development, with particular expertise in high-energy-density physics, laser science, high-performance computing and science/engineering at the nanometer/subpicosecond scale, LLNL innovations improve security, meet energy and environmental needs and strengthen U.S. economic competitiveness. The Laboratory also partners with other research institutions, universities and industry to bring the full weight of the nation's science and technology community to bear on solving problems of national importance.

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