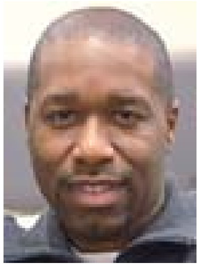

Jefferson Lab's Leon Cole

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DOE Pulse

Science and Technology Highlights from the DOE National Laboratories

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Research Highlights . . .

Free-Electron Laser targets fat

Fat may have finally met its match: laser light. Researchers at the Wellman Center for Photomedicine at Massachusetts General Hospital, Harvard Medical School and the Free-Electron Laser at the Department of Energy's Jefferson Lab have shown, for the first time, that a laser can preferentially heat lipid-rich tissues, or fat, in the body without harming the overlying skin. Laser therapies based on the new research could treat a variety of health conditions, including severe acne, atherosclerotic plaque, and unwanted cellulite. The result was presented at the American Society for Laser Medicine and Surgery (ASLMS) 26th Annual Meeting in Boston, Mass.

[Kandice Carter, 757/269-7263, kcarter@jlab.org]

Argonne has finest-focused X-rays

A device developed at DOE's Argonne National Laboratory has set a world's record for tiny spot size with a hard X-ray beam. The device is called a Multilayer Laue Lens. Enhancements to the device have now increased its ability to focus the X-rays with an energy level of 19.5 keV to 30 nanometers. The lens allows precise focusing of the X-ray light, allowing analysis of electronic circuit boards or samples inside high-pressure or high-temperature cells. Argonne researchers developed the record-setting lens by depositing 728 layers of material, one layer at a time, on a silicon substrate wafer. The thickness of the layer stack, when completed, was 12.4 microns.

[Catherine Foster, 630/252-5580, cfoster@anl.gov]

Shrinking Magnetic Storage Media to the Nanoscale

In the world of electronics, the smaller the space one bit of information can occupy, the more data you can get into a device and the faster it can operate. In a step toward shrinking magneto-electronic devices down to the nanoscale, or billionths of a meter, scientists at Brookhaven Lab have fabricated patterned films of 100-nanometer magnetic dots. The scientists are seeking to understand the mechanism by which the polarities of individual dots can be reversed at will without interference. If they identify two distinct, stable states, these could be used to represent or record the "ones" and "zeros" of digital code.

[Karen McNulty Walsh, 631/344-8350, kmcnulty@bnl.gov]

Nanoscale drug delivery system

Delivering a dose of chemotherapy drugs to specific cancer cells without the risk of side affects to healthy cells may one day be possible thanks to a nanoscale drug delivery system being explored by researcher Victor Lin at DOE's Ames Laboratory. Using tiny silica particles call mesoporous nanospheres to carry drugs inside living cells, Lin is studying different methods to control whether or not the particle delivers its pharmaceutical payload. The nanospheres have thousands of parallel channels running completely through them that can be "capped" to safely seal the drug inside. Once the nanospheres are inside the target cells, a trigger is used to pop the caps off and release the drug.

[Kerry Gibson, 515/294-1405, kgibson@ameslab.gov]

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/) is distributed every two weeks. For more information, please contact Jeff Sherwood (jeff.sherwood@hq.doe.gov, 202-586-5806).

A "Tool" de Force

Ames Laboratory's Mark Gordon has devoted much of his professional career to making sure the right tools are available in GAMESS, the "toolbox" that he and thousands of researchers worldwide use on a daily basis to learn more about the goings-on of molecules and atoms--how they act, interact and react.

GAMESS, or the General Atomic and Molecular Electronic Structure System, is a software suite chock-full of quantum chemistry codes--tools that take advantage of parallel, high-performance supercomputing systems to perform the very highest levels of theory required to help solve problems related to combustion, catalysis, photochemical energy conversion and the design of new fuels.

Gordon cultivates the GAMESS software tools through mentoring graduate students and collaborating with his numerous professional colleagues. One of the GAMESS tools, the Fragment Molecular Orbital, or FMO method, was developed for GAMESS by Gordon's former graduate student, Dimitri Fedorov, and his colleague, Kazuo Kitaura, both of the Japanese National Computational Laboratory, AIST. The FMO method solves the problem of doing quantum chemistry on a large molecule, such as a polymer, enzyme or protein, by "chopping" it into small pieces, doing calculations on those pieces, and then uniting the fragments to make the larger system.

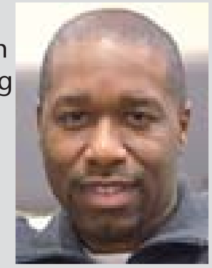
To enhance the FMO tool, Gordon led a team that included his postdoctoral researcher, Hui Li; former graduate student, Jan Jensen, now at the University of Iowa; Fedorov; and Kitaura in developing a method of modeling the activity of molecules in solution. They created the new GAMESS tool by interfacing the Polarizable Continuum Model, PCM, with the FMO method. "If you're interested in polymers and enzymes, whatever they do, they do in solution," says Gordon. "That means just doing FMO calculations is not enough—you need to get the solvent in there."

Li, who will be an assistant professor next fall at the University of Nebraska, and Netzloff, now at Australian National University, respectively created a molecular dynamics code to address the interactions that occur between ions and optimized the code to take advantage of parallel computers. The addition of the charge transfer code to GAMESS is of particular importance to Gordon who is interested in ionic liquids in the design of high-energy fuels--products that bring together positively and negatively charged species. "You can't simulate those relationships adequately unless you have something that accounts for the charge transfer interactions, and we now have that capability in GAMESS," says Gordon.

GAMESS is distributed at no cost to users by accessing www.msg.ameslab.gov and signing a license agreement.

Submitted by DOE's Ames Laboratory

Student studies strange matter



Leon Cole

Leon Cole is looking at strange matter. He's working on an experiment that's attempting to create and study lambda hyperons, particles similar to protons and neutrons. It's thought that lambda hyperons are an essential ingredient of neutron stars.

Cole is a graduate student at Hampton University in Hampton, Va. and is busy working on his Ph.D. thesis research at Jefferson Lab. He says while protons and neutrons both contain three quarks consisting of the up and down varieties, "This lambda particle contains an up, a down, and a strange quark."

Studying how lambdas interact with ordinary protons and neutrons inside the nucleus may help scientists understand more about how protons and neutrons are glued together.

It's a far cry from the career Cole thought he'd have. Originally from Camden, Ala., Cole attended Jackson State University in Jackson, Miss, majoring in electrical engineering. Those plans changed with a research opportunity at Jefferson Lab the summer after his freshman year. The opportunity prompted Cole to change his major to physics and has led to stints at both MIT-Bates and Fermilab.

He says he's glad he made the switch. "I can't see the nucleus of the atom; I can't physically put my hand on it. And yet, we can create experiments to study the inside of the nucleus. As small as it is - we can do it."

Away from the Lab, Cole enjoys bowling, reading, and solving jigsaw puzzles. He has also mentored a Cub Scout troop in nearby Newport News. He says he'd like to one day continue his role as a mentor for young physics students.

"Even though we've learned a lot from scientists before us, I think there's still a lot more to learn. So hopefully, I can be a part of that new frontier of scientists that pushes us forward," he says.

Submitted by DOE's Jefferson Lab