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NERSC National Energy Research Scientific Computing Center

BERKELEY LAB Lawrence Berkeley National Laboratory

A BETTER LITHIUM-ION BATTERY ON THE WAY

Simulations Reveal How New Polymer Absorbs Eight Times the Lithium of Current Designs

SEPTEMBER 23, 2011
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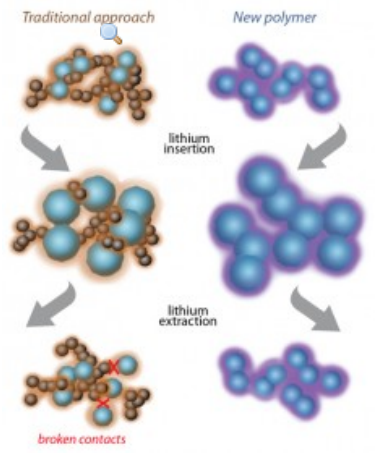
Lithium-ion batteries are everywhere, in smart phones, laptops, an array of other consumer electronics, and the newest electric cars. Good as they are, they could be much better, especially when it comes to lowering the cost and extending the range of electric cars. To do that, batteries need to store a lot more energy.

A team of scientists at the U.S. Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) has designed a new kind of anode — a critical energy-storing component — capable of absorbing eight times the lithium of current designs. The new type anode has maintained its greatly increased energy capacity after over a year of testing and many hundreds of charge-discharge cycles.

The secret is a tailored polymer that conducts electricity and binds closely to lithium-storing silicon particles, even as they expand to more than three times their volume during charging and then shrink again during discharge. The new anodes are made from low-cost materials, compatible with standard lithium-battery manufacturing technologies. Using supercomputers at the National Energy Research Scientific Computing Center (NERSC), the team ran *ab initio* calculations of the promising polymers until they achieved this result. The research team reports its findings in *Advanced Materials*, now available online.

"We had the experimental evidence, but to understand what we were seeing, and its relevance to the conductivity of the polymer, we needed a theoretical explanation, starting from first principles," says Wanli Yang of Berkeley Lab's Advanced Light Source (ALS).



At left, the traditional approach to composite anodes using silicon (blue spheres) for higher energy capacity has a polymer binder such as PVDF (light brown) plus added particles of carbon to conduct electricity (dark brown spheres). Silicon swells and shrinks while acquiring and releasing lithium ions, and repeated swelling and shrinking eventually break contacts among the conducting carbon particles. At right, the new Berkeley Lab polymer (purple) is itself conductive and continues to bind tightly to the silicon particles despite repeated swelling and shrinking.

High-capacity expansion

"High-capacity lithium-ion anode materials have always confronted the challenge of volume change – swelling – when electrodes absorb lithium," says Gao Liu of Berkeley Lab's Environmental Energy Technologies Division (EETD), a member of the BATT program (Batteries for Advanced Transportation Technologies) managed by the Lab and supported by DOE's Office of Vehicle Technologies.

Says Liu, "Most of today's lithium-ion batteries have anodes made of graphite, which is electrically conducting and expands only modestly when housing the ions between its graphene layers. Silicon can store 10 times more – it has by far the highest capacity among lithium-ion storage materials – but it swells to more than three times its volume when fully charged."

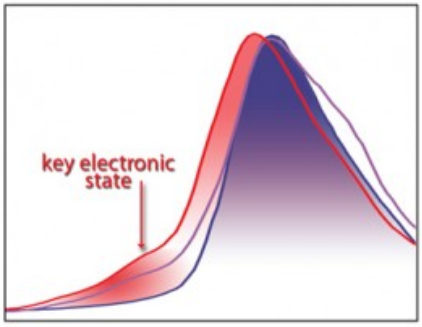
This kind of swelling quickly breaks the electrical contacts in the anode, so researchers have concentrated on finding other ways to use silicon while maintaining anode conductivity. Many approaches have been proposed; some are prohibitively costly.

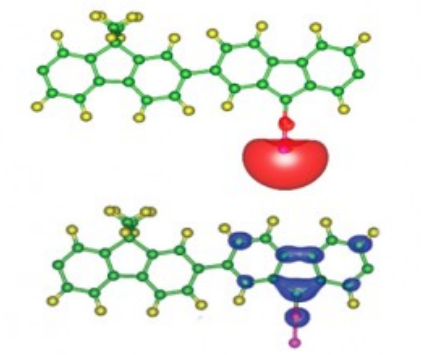
One less-expensive approach has been to mix silicon particles in a flexible polymer binder, with carbon black added to the mix to conduct electricity. Unfortunately, the repeated swelling and shrinking of the silicon particles as they acquire and release lithium ions eventually push away the added carbon particles. What's needed is a flexible binder that can conduct electricity by itself, without the added carbon.

"Conducting polymers aren't a new idea," says Liu, "but previous efforts haven't worked well, because they haven't taken into account the severe reducing environment on the anode side of a lithium-ion battery, which renders most conducting polymers insulators."

One such experimental polymer, called PAN (polyaniline), has positive charges; it starts out as a conductor but quickly loses conductivity. An ideal conducting polymer should readily acquire electrons, rendering it conducting in the anode's reducing environment.

The signature of a promising polymer would be one with a low value of the state called the "lowest unoccupied molecular orbital," where electrons can easily reside and move freely. Ideally, electrons would be acquired from the lithium atoms during the initial charging process. Liu and his postdoctoral fellow Shidi Xun in EETD designed a series of such polyfluorene-based conducting polymers – PFs for short.





At top, spectra of a series of polymers obtained with soft x-ray absorption spectroscopy at ALS beamline 8.0.1 show a lower "lowest unoccupied molecular orbital" for the new Berkeley Lab polymer, PFFOMB (red), than other polymers (purple), indicating better potential conductivity. Here the peak on the absorption curve reveals the lower key electronic state. At bottom, simulations disclose the virtually complete, two-stage electron charge transfer when lithium ions bind to the new polymer.

When Liu discussed the excellent performance of the PFs with Wanli Yang of Berkeley Lab's Advanced Light Source (ALS), a scientific collaboration emerged to understand the new materials. Yang suggested conducting soft x-ray absorption spectroscopy on Liu and Xun's candidate polymers using ALS beamline 8.0.1 to determine their key electronic properties.

Says Yang, "Gao wanted to know where the ions and electrons are and where they move. Soft x-ray spectroscopy has the power to deliver exactly this kind of crucial information."

Compared with the electronic structure of PAN, the absorption spectra Yang obtained for the PFs stood out immediately. The differences were greatest in PFs incorporating a carbon-oxygen functional group (carbonyl).

"We had the experimental evidence," says Yang, "but to understand what we were seeing, and its relevance to the conductivity of the polymer, we needed a theoretical explanation, starting from first principles." He asked Lin-Wang Wang of Berkeley Lab's Materials Sciences Division (MSD) to join the research collaboration.

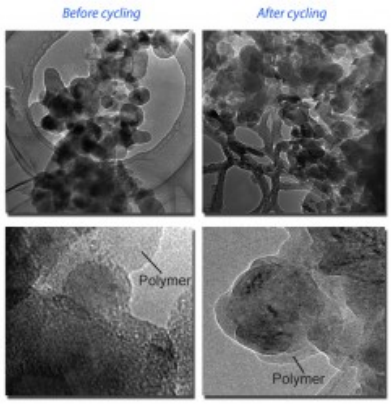
Wang and his postdoctoral fellow, Nenad Vukmirovic, conducted *ab initio* calculations of the promising polymers at the Lab's National Energy Research Scientific Computing Center (NERSC). Wang says, "The calculation tells you what's really going on – including precisely how the lithium ions attach to the polymer, and why the added carbonyl functional group improves the process. It was quite impressive that the calculations matched the experiments so beautifully."

The simulation did indeed reveal "what's really going on" with the type of PF that includes the carbonyl functional group, and showed why the system works so well. The lithium ions interact with the polymer first, and afterward bind to the silicon particles. When a lithium atom binds to the polymer through the carbonyl group, it gives its electron to the polymer – a doping process that significantly improves the polymer's electrical conductivity, facilitating electron and ion transport to the silicon particles.

Cycling for success

Having gone through one cycle of material synthesis at EETD, experimental analysis at the ALS, and theoretical simulation at MSD, the positive results triggered a new cycle of improvements. Almost as important as its electrical properties are the polymer's physical properties, to which Liu now added another functional group, producing a polymer that can adhere tightly to the silicon particles as they acquire or lose lithium ions and undergo repeated changes in volume.

Scanning electron microscopy and transmission electron microscopy at the National Center for Electron Microscopy (NCEM), showing the anodes after 32 charge-discharge cycles, confirmed that the modified polymer adhered strongly throughout the battery operation even as the silicon particles repeatedly expanded and contracted. Tests at the ALS and simulations confirmed that the added mechanical properties did not affect the polymer's superior electrical properties.



Transmission electron microscopy reveals the new conducting polymer's improved binding properties. At left, silicon particles embedded in the binder are shown before cycling through charges and discharges (closer view at bottom). At right, after 32 charge-discharge cycles, the polymer is still tightly bound to the silicon particles, showing why the energy capacity of the new anodes remains much higher than graphite anodes after more than 650 charge-discharge cycles during testing.

"Without the input from our partners at the ALS and in MSD, what can be modified and what should not be modified in the next generation of polymers would not have been obvious," says Vince Battaglia, Program Manager of EETD's Advanced Energy Technologies Department.

"This achievement provides a rare scientific showcase, combining advanced tools of synthesis, characterization, and simulation in a novel approach to materials development," says Zahid Hussain, the ALS Division Deputy for Scientific Support and Scientific Support Group Leader. "The cyclic approach can lead to the discovery of new practical materials with a fundamental understanding of their properties."

The icing on the anode cake is that the new PF-based anode is not only superior but economical. "Using commercial silicon particles and without any conductive additive, our composite anode exhibits the best performance so far," says Gao Liu. "The whole manufacturing process is low cost and compatible with established manufacturing technologies. The commercial value of the polymer has already been recognized by major companies, and its possible applications extend beyond silicon anodes."

Anodes are a key component of lithium-ion battery technology, but far from the only challenge. Already the research collaboration is pushing to the next step, studying other battery components including cathodes.

"Polymers with Tailored Electronic Structure for High Capacity Lithium Battery Electrodes," by Gao Liu, Shidi Xun, Nenad Vukmirovic, Xiangyun Song, Paul Olalde-Velasco, Honghe Zheng, Vince S. Battaglia, Lin-Wang Wang, and Wanli Yang, appears in Advanced Materials and is available online at ***http://onlinelibrary.wiley.com/doi/10.1002/adma.201102421/abstract***.

Materials research for this work in the BATT program was supported by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy. The ALS, NCEM, and NERSC are national scientific user facilities supported by DOE's Office of Science.

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ACCELERATING ADVANCED MATERIAL DEVELOPMENT

NERSC Science Gateway a 'Google of Material Properties'

OCTOBER 31, 2011 | Tags: Materials Science, Science Gateways
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New materials are crucial to building a clean energy economy—for everything from batteries to photovoltaics to lighter weight vehicles—but today the development cycle is too slow: around 18 years from conception to commercialization. To speed up this process, a team of researchers from the Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and the Massachusetts Institute of Technology (MIT) teamed up to develop a new computational tool. Called the Materials Project, it launches this month.

Kristin Persson is one of the founding scientists behind the Materials Project, a computational tool aimed at taking the guesswork out of new materials discoveries, especially those aimed at energy applications like batteries. (Roy Kaltschmidt, LBNL)

The tool, which sits on the National Energy Research Scientific Computing Center's (NERSC) science gateway infrastructure, was developed with support from the Department of Energy and a Laboratory Directed Research and Development Grant from Berkeley Lab.

"Our vision is for this tool to become a dynamic 'Google' of material properties, which continually grows and changes as more users come on board to analyze the results, verify against experiments and increase their knowledge," says Kristin Persson, a Berkeley Lab chemist and one of the founding scientists behind the Materials Project. "So many scientists can benefit from this type of screening. Considering the demand for innovative clean energy technology, we needed most of these materials yesterday."

Taking a Genome-like Approach

The Materials Project employs an approach to materials science inspired by genomics. But rather than sequencing genomes, researchers are using supercomputers to characterize the properties of inorganic compounds, such as their stability, voltage, capacity, and oxidation state. The results are then organized into a database with a user-friendly web interface that gives all researchers free and easy access and searching.

"First-principles calculations have reached the point of accuracy where many materials properties, relevant for photovoltaics, batteries and thermoelectrics, can be reliably predicted," says Gerbrand Ceder, an MIT professor of materials science and engineering and founder of the Materials Project.

A better battery—one that is cheaper and has more power and energy while being safe—could finally make possible the dream of an electric vehicle reaching performance and cost parity with a gasoline-powered car. But beyond batteries, novel materials could transform a host of other industries, from food packaging to buildings. For example, the Materials Project is working with several entities interested in making stronger, corrosion-resistant, lightweight aluminium alloys, which could make possible lighter vehicles and airplanes.

"Materials innovation today is largely done by intuition, which is based on the experience of single investigators," says Persson, who works in Berkeley Lab's Environmental Energy Technologies Division. "The lack of comprehensive knowledge of materials, organized for easy analysis and rational design, is one of the foremost reasons for the long process time in materials discovery."

President Obama has recognized the importance of advanced materials with his announcement in June of the Materials Genome Initiative "to double the speed with which we discover, develop, and manufacture new materials." Many of the concepts of that initiative were inspired by the Materials Project, Persson said.

With the help of supercomputers at the Department of Energy's NERSC, the Berkeley Lab Lawrencium cluster and systems at the University of Kentucky, the Materials Project database currently contains the structural and energetic properties of more than 15,000 inorganic compounds, and up to hundreds more are added every day. Researchers are continuously adding new properties to enable true rational design of new materials for a wide variety of applications.

A Gateway for Science

To build the Materials Project web tool, the team approached computer systems engineers at NERSC who have extensive experience building web-based interfaces and technologies. These science gateways make it easier for researchers to access computational resources and share data with the rest of their community.

"The Materials Project represents the next generation of the original Materials Genome Project, developed by Ceder's team at MIT," says Shreyas Cholia, a NERSC computer engineer who helped develop the Materials Project tool. "The core science team worked with developers from NERSC and Berkeley Lab's Computational Research Division to expand this tool into a more permanent, flexible and scalable data service built on top of rich modern web interfaces and state-of-the-art NoSQL database technology."

The Materials Project, which will be hosted on NERSC's science gateway infrastructure, was developed with support from the Department of Energy and a Laboratory Directed Research and Development grant from Berkeley Lab.

In addition to Persson and Cholia, other Berkeley Lab contributors to this project include Michael Kocher, Daniel Gunter, Annette Greiner, David Skinner and David Bailey. MIT collaborators include Gerbrand Ceder, Shyue Ping Ong, Anubhav Jain, Geoffroy Hautier and Evgueni Chtykov.

“At NERSC we have a long history of engaging with science teams to create web-based tools that allow scientists to share and access data, perform computations and interact with NERSC systems using web-based technologies, so it was a perfect match,” adds Cholia.

Research teams interested in initiating their own science gateway projects at NERSC should contact David Skinner at **deskinner@lbl.gov**.

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CALCULATING WHAT'S IN THE UNIVERSE FROM THE BIGGEST COLOR 3-D MAP

Berkeley Lab scientists and their Sloan Digital Sky Survey colleagues use galactic brightness to build a precision model of the cosmos

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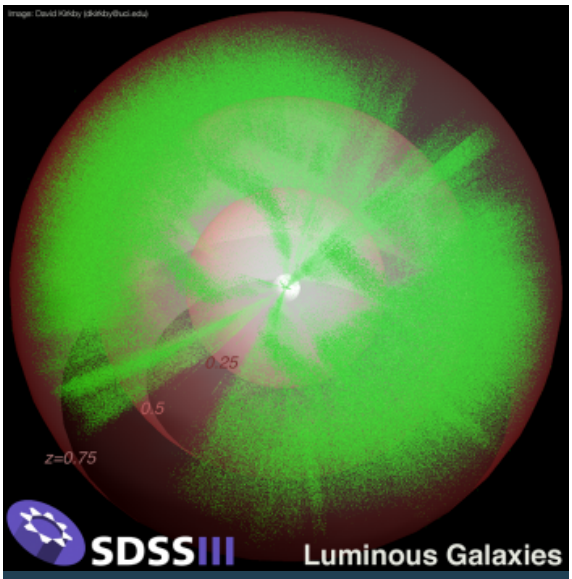
Since 2000, the three Sloan Digital Sky Surveys (SDSS I, II, III) have surveyed well over a quarter of the night sky and produced the biggest color map of the universe in three dimensions ever. Now scientists at the U.S. Department of Energy's Lawrence Berkeley National Laboratory (Berkeley Lab) and their SDSS colleagues, working with DOE's National Energy Research Scientific Computing Center (NERSC) based at Berkeley Lab, have used this visual information for the most accurate calculation yet of how matter clumps together – from a time when the universe was only half its present age until now.



This image shows over a million luminous galaxies at redshifts indicating times when the universe was between seven and eleven billion years old, from which the sample in the current studies was selected. (By David Kirkby of the University of California at Irvine and the SDSS collaboration.)

"The way galaxies cluster together over vast expanses of the sky tells us how both ordinary visible matter and underlying invisible dark matter are distributed, across space and back in time," says Shirley Ho, an astrophysicist at Berkeley Lab and Carnegie Mellon University, who led the work. "The distribution gives us cosmic rulers to measure how the universe has expanded, and a basis for calculating what's in it: how much dark matter, how much dark energy, even the mass of the hard-to-see neutrinos it contains. What's left over is the ordinary matter and energy we're familiar with."

For the present study Ho and her colleagues first selected 900,000 luminous galaxies from among over 1.5 million such galaxies gathered by the Baryon Oscillation Spectrographic Survey, or BOSS, the largest component of the still-ongoing SDSS III. Most of these are ancient red galaxies, which contain only red stars because all their faster-burning stars are long gone, and which are exceptionally bright and visible at great distances. The galaxies chosen for this study populate the largest volume of space ever used for galaxy clustering measurements. Their brightness was measured in five different colors, allowing the redshift of each to be estimated.

"By covering such a large area of sky and working at such large distances, these measurements are able to probe the clustering of galaxies on incredibly vast scales, giving us unprecedented constraints on the expansion history, contents, and evolution of the universe," says Martin White of Berkeley Lab's Physics Division, a professor of physics and astronomy at the University of California at Berkeley and chair of the BOSS science survey teams. "The clustering we're now measuring on the largest scales also contains vital information about the origin of the structure we see in our maps, all the way back to the epoch of inflation, and it helps us to constrain – or rule out – models of the very early universe."

After augmenting their study with information from other data sets, the team derived a number of such cosmological constraints, measurements of the universe's contents based on different cosmological models. Among the results: in the most widely accepted model, the researchers found – to less than two percent uncertainty – that dark energy accounts for 73 percent of the density of the universe.

The team's results are presented January 11 at the annual meeting of the American Astronomical Society in Austin, Texas, and have been submitted to the Astrophysical Journal. They are currently available online at http://arxiv.org/abs/1201.2137.

The power of the universe

"The way mass clusters on the largest scales is graphed in an angular power spectrum, which shows how matter statistically varies in density across the sky," says Ho. "The power spectrum gives a wealth of information, much of which is yet to be exploited." For example, information about inflation – how the universe rapidly expanded shortly after the big bang – can be derived from the power spectrum.

Closely related to the power spectrum are two "standard rulers," which can be used to measure the history of the expansion of the universe. One ruler has only a single mark – the time when matter and radiation were exactly equal in density.

"In the very early universe, shortly after the big bang, the universe was hot and dominated by photons, the fundamental particles of radiation," Ho explains. "But as it expanded,

it began the transition to a universe dominated by matter. By about 50,000 years after the big bang, the density of matter and radiation were equal. Only when matter dominated could structure form."

The other cosmic ruler is also big, but it has many more than one mark in the power spectrum; this ruler is called BAO, for baryon acoustic oscillations. (Here, baryon is shorthand for ordinary matter.) Baryon acoustic oscillations are relics of the sound waves that traveled through the early universe when it was a hot, liquid-like soup of matter and photons. After about 50,000 years the matter began to dominate, and by about 300,000 years after the big bang the soup was finally cool enough for matter and light to go their separate ways.

Differences in density that the sound waves had created in the hot soup, however, left their signatures as statistical variations in the distribution of light, detectable as temperature variations in the cosmic microwave background (CMB), and in the distribution of baryons. The CMB is a kind of snapshot that can still be read today, almost 14 billion years later. Baryon oscillations – variations in galactic density peaking every 450 million light-years or so – descend directly from these fluctuations in the density of the early universe.

BAO is the target of the Baryon Oscillation Spectroscopic Survey. By the time it's completed, BOSS will have measured the individual spectra of 1.5 million galaxies, a highly precise way of measuring their redshifts. The first BOSS spectroscopic results are expected to be announced early in 2012.

Meanwhile the photometric study by Ho and her colleagues deliberately uses many of the same luminous galaxies but derives redshifts from their brightnesses in different colors, extending the BAO ruler back over a previously inaccessible redshift range, from z = 0.45 to z = 0.65 (z stands for redshift).

"As an oscillatory feature in the power spectrum, not many things can corrupt or confuse BAO, which is why it is considered one of the most trustworthy ways to measure dark energy," says Hee-Jong Seo of the Berkeley Center for Cosmological Physics at Berkeley Lab and the UC Berkeley Department of Physics, who led BAO measurement for the project. "We call BAO a standard ruler for a good reason. As dark energy stretches the universe against the gravity of dark matter, more dark energy places galaxies at a larger distance from us, and the BAO imprinted in their distribution looks smaller. As a standard ruler the true size of BAO is fixed, however. Thus the apparent size of BAO gives us an estimate of the cosmological distance to our target galaxies – which in turn depends on the properties of dark energy."

Says Ho, "Our study has produced the most precise photometric measurement of BAO. Using data from the newly accessible redshift range, we have traced these wiggles back to when the universe was about half its present age, all the way back to z = 0.54."

Seo adds, "And that's to an accuracy within 4.5 percent."

Reining in the systematics

"With such a large volume of the universe forming the basis of our study, precision cosmology was only possible if we could control for large-scale systematics," says Ho. Systematic errors are those with a physical basis, including differences in the brightness of the sky, or stars that mimic the colors of distant galaxies, or variations in weather affecting "seeing" at the SDSS's Sloan Telescope – a dedicated 2.5 meter telescope at the Apache Point Observatory in southern New Mexico.

After applying individual corrections to these and other systematics, the team cross-correlated the effects on the data and developed a novel procedure for deriving the best angular power-spectrum of the universe with the lowest statistical and systematic errors.

With the help of 40,000 central-processing-unit (CPU) hours at NERSC and another 20,000 CPU hours on the Riemann computer cluster at Berkeley Lab, NERSC's powerful computers and algorithms enabled the team to use all the information from galactic clustering in a huge volume of sky, including the full shape of the power spectrum and, independently, BAO, to get excellent cosmological constraints. The data as well as the analysis output are stored at NERSC.

"Our dataset is purely imaging data, but our results are competitive with the latest large-scale spectroscopic surveys," Ho says. "What we lack in redshift precision, we make up in sheer volume. This is good news for future imaging surveys like the Dark Energy Survey and the Large Synoptic Survey Telescope, suggesting they can achieve significant cosmological constraints even compared to future spectroscopy surveys."

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Animated visualizations of the luminous galaxies in the SDSS-III dataset can be accessed at **http://darkmatter.ps.uci.edu/lrg-sdss**.

"Clustering of Sloan Digital Sky Survey III photometric luminous galaxies: The measurement, systematics, and cosmological implications," by Shirley Ho, Antonio Cuesta, Hee-Jong Seo, Roland de Putter, Ashley J. Ross, Martin White, Nikhil Padmanabhan, Shun Saito, David J. Schlegel, Eddie Schlafly, Uroš Seljak, Carlos Hernández-Monteagudo, Ariel G. Sánchez, Will J. Percival, Michael Blanton, Ramin Skibba, Don Schneider, Beth Reid, Olga Mena, Matteo Viel, Daniel J. Eisenstein, Francisco Prada, Benjamin Weaver, Neta Bahcall, Dimitry Bizyaev, Howard Brewinton, Jon Brinkman, Luiz Nicolaci da Costa, John R. Gott, Elena Malanushenko, Viktor Malanushenko, Bob Nichol, Daniel Oravetz, Kaike Pan, Nathalie Palanque-Delabrouille, Nicholas P. Ross, Audrey Simmons, Fernando de Simoni, Stephanie Snedden,and Christophe Yeche, has been submitted to Astrophysical Journal and is now available online at **http://arxiv.org/abs/1201.2137**.

"Acoustic scale from the angular power spectra of SDSS-III DR8 photometric luminous galaxies," by Hee-Jong Seo, Shirley Ho, Martin White, Antonio J. Cuesta, Ashley J. Ross, Shun Saito, Beth Reid, Nikhil Padmanabhan, Will J. Percival, Roland de Putter, David J. Schlegel, Daniel J. Eisenstein, Xiaoying Xu, Donald P. Schneider, Ramin Skibba, Licia Verde, Robert C. Nichol, Dmitry Bizyaev, Howard Brewington, J. Brinkmann, Luiz Alberto Nicolai da Costa, J. Richard Gott III, Elena Malanushenko, Viktor Malanushenko, Dan Oravetz, Nathalie Palanque-Delabrouille, Kaike Pan, Francisco Prada, Nicholas P. Ross, Audrey Simmons, Fernando Simoni, Alaina Shelden, Stephanie Snedden, and Idit Zehavi, has been submitted to Astrophysical Journal and is available online at **http://arxiv.org/abs/1201.2172**.

Funding for SDSS-III has been provided by the Alfred P. Sloan Foundation, the Participating Institutions, the National Science Foundation, and the U.S. Department of Energy's Office of Science. The SDSS-III web site is **http://www.sdss3.org**/.

SDSS-III is managed by the Astrophysical Research Consortium for the Participating Institutions of the SDSS-III Collaboration including the University of Arizona, the Brazilian Participation Group, Brookhaven National Laboratory, University of Cambridge, Carnegie Mellon University, University of Florida, the French Participation Group, the German Participation Group, the Instituto de Astrofisica de Canarias, the Michigan State/Notre Dame/JINA Participation Group, Johns Hopkins University, Lawrence Berkeley National Laboratory, Max Planck Institute for Astrophysics, New Mexico State University, New York University, Ohio State University, Pennsylvania State University, University of Portsmouth, Princeton University, the Spanish Participation Group, University of Tokyo, University of Utah, Vanderbilt University, University of Virginia, University of Washington, and Yale University.

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Clearest Picture Yet of Dark Matter Points the Way to Better Understanding of Dark Energy

Posted By paulpreuss On January 9, 2012 @ 1:00 pm In News Releases | Comments Disabled

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BATAVIA, Illinois, and BERKELEY, California –Two teams of physicists at the U.S. Department of Energy's Fermilab and Lawrence Berkeley National Laboratory (Berkeley Lab) have independently made the largest direct measurements of the invisible scaffolding of the universe, building maps of dark matter using new methods that, in turn, will remove key hurdles for understanding dark energy with ground-based telescopes.

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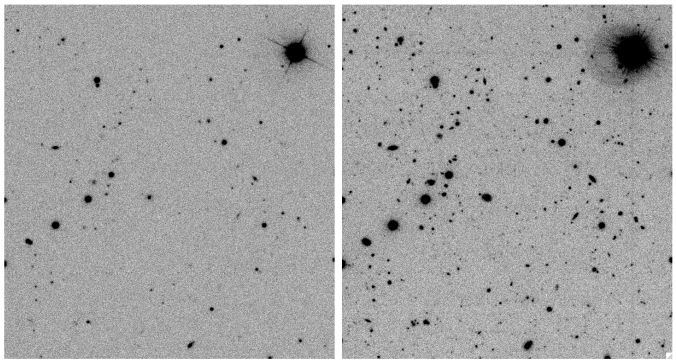
Teams from Fermilab and Berkeley Lab used galaxies from wide-ranging SDSS Stripe 82, a tiny detail of which is shown here, to plot new maps of dark matter based on the largest direct measurements of cosmic shear to date. (Image credit SDSS)

The teams' measurements look for tiny distortions in the images of distant galaxies, called "cosmic shear," caused by the gravitational influence of massive, invisible dark matter structures in the foreground. Accurately mapping out these dark-matter structures and their evolution over time is likely to be the most sensitive of the few tools available to physicists in their ongoing effort to understand the mysterious space-stretching effects of dark energy.

Both teams depended upon extensive databases of cosmic images collected by the Sloan Digital Sky Survey (SDSS), which were compiled in large part with the help of Berkeley Lab and Fermilab.

"These results are very encouraging for future large sky surveys. The images produced lead to a picture that sees many more galaxies in the universe and sees those that are six time fainter, or further back in time, than is available from single images," says Huan Lin, a Fermilab physicist and member of the SDSS and the Dark Energy Survey (DES) .

Melanie Simet, a member of the SDSS collaboration from the University of Chicago, will outline the new techniques for improving maps of cosmic shear and explain how these techniques can expand the reach of upcoming international sky survey experiments during a talk at 2 p.m. CST on Monday, January 9, at the American Astronomical Society (AAS) conference in Austin, Texas. In her talk she will demonstrate a unique way to analyze dark matter's distortion of galaxies to get a better picture of the universe's past.



[5]

Layering photos of one area of sky taken at various time periods, a process called coaddition, can increase the sensitivity of the images six-fold, by removing errors and enhancing faint light signals. The image on the left shows a single picture of galaxies from SDSS Stripe 82. The image on the right shows the same area after layering, increasing the number of visible, distant galaxies. (Image credit SDSS)

Eric Huff, an SDSS member from Berkeley Lab and the University of California at Berkeley, will present a poster describing the full cosmic shear measurement, including the new constraints on dark energy, from 9 a.m. to 2 p.m. CST on Thursday, January 12, at the AAS conference.

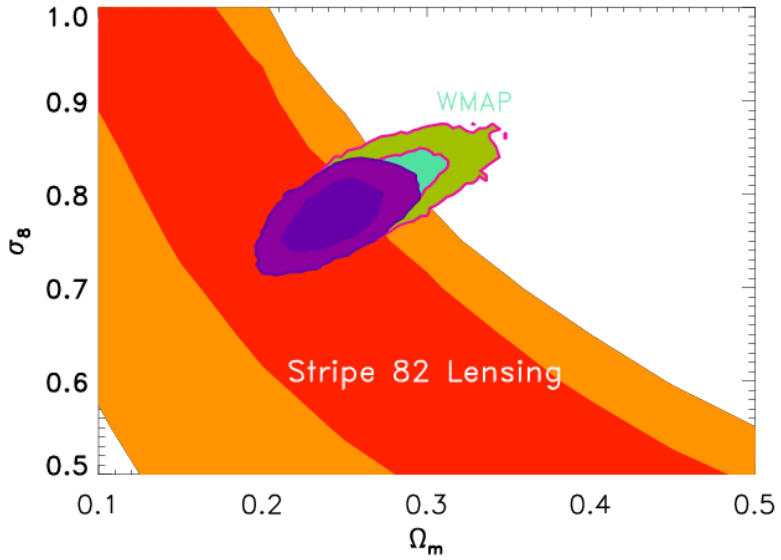
Several large astronomical surveys, such as the Dark Energy Survey, the Large Synoptic Survey Telescope, and the HyperSuprimeCam survey, will try to measure cosmic shear in the coming years. Weak lensing distortions are so subtle, however, that the same atmospheric effects that cause stars to twinkle at night pose a formidable challenge for cosmic shear measurements. Until now, no ground-based cosmic-shear measurement has been able to completely and provably separate weak lensing effects from the atmospheric distortions.

"The community has been building towards cosmic shear measurements for a number of years now," says Huff, an astronomer at Berkeley Lab, "but there's also been some skepticism as to whether they can be done accurately enough to constrain dark energy. Showing that we can achieve the required accuracy with these pathfinding studies is important for the next generation of large surveys."

To construct dark matter maps, the Berkeley Lab and Fermilab teams used images of galaxies collected between 2000 and 2009 by SDSS surveys I and II, using the Sloan Telescope at Apache Point Observatory in New Mexico. The galaxies lie within a continuous ribbon of sky known as SDSS Stripe 82, lying along the celestial equator and encompassing 275 square degrees. The galaxy images were captured in multiple passes over many years.

The two teams layered snapshots of a given area taken at different times, a process called coaddition, to remove errors caused by the atmospheric effects and to enhance very faint signals coming from distant parts of the universe. The teams used different techniques to model and control for the atmospheric variations and to measure the lensing signal, and have performed an exhaustive series of tests to prove that these models work.

Gravity tends to pull matter together into dense concentrations, but dark energy acts as a repulsive force that slows down the collapse. Thus the clumpiness of the dark matter maps provides a measurement of the amount of dark energy in the universe.



When they compared their final results before the AAS meeting, both teams found somewhat less structure than would have been expected from other measurements such as the Wilkinson Microwave Anisotropy Probe (WMAP), but, says Berkeley Lab's Huff, "the results are not yet different enough from

previous experiments to ring any alarm bells."

Meanwhile, says Fermilab's Lin, "Our image-correction processes should prove a valuable tool for the next generation of weak-lensing surveys."

[6]

Constraints on cosmological parameters from SDSS Stripe 82 cosmic shear at the 1- and 2-sigma level. Also shown are the constraints from WMAP. The innermost region is the combined constraint from both WMAP and Stripe 82. (Image credit SDSS)

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This is a joint release of Fermilab and Berkeley Lab. Fermilab's release is posted at http://www.fnal.gov/pub/presspass/press_releases/2012/Dark-Energy-20120109.html [7]

Fermilab and University of Chicago scientific papers related to these results are accessible online at the following sites:

- coadd data: http://arxiv.org/abs/1111.6619 [8]
- photometric redshifts: http://arxiv.org/abs/1111.6620 [9]
- cluster lensing: http://arxiv.org/abs/1111.6621 [10]
- cosmic shear: http://arxiv.org/abs/1111.6622 [11]

Berkeley Lab and University of California at Berkeley scientific papers related to these results are accessible online at:

- coadd data: http://arxiv.org/abs/1111.6958 [12]
- cosmic shear: http://arxiv.org/abs/1112.3143 [13]

Lawrence Berkeley National Laboratory addresses the world's most urgent scientific challenges by advancing sustainable energy, protecting human health, creating new materials, and revealing the origin and fate of the universe. Founded in 1931, Berkeley Lab's scientific expertise has been recognized with 13 Nobel prizes. The University of California manages Berkeley Lab for the U.S. Department of Energy's Office of Science. For more, visit www.lbl.gov [14].

Fermilab is a national laboratory supported by the Office of Science of the U.S. Department of Energy, operated under contract by Fermi Research Alliance, LLC. Visit Fermilab's website at http://www.fnal.gov [15].

The DOE Office of Science is the single largest supporter of basic research in the physical sciences in the United States, and is working to address some of the most pressing challenges of our time. For more information, please visit http://science.energy.gov [16].

The National Science Foundation supported this research. For more information, please visit http://www.nsf.gov/ [17].

The Sloan Digital Sky Survey is the most ambitious survey of the sky ever undertaken, involving more than 300 astronomers and engineers at 25 institutions around the world. SDSS-II, which began in 2005 and finished observations in July, 2008, is comprised of three complementary projects.

Funding for the SDSS and SDSS-II has been provided by the Alfred P. Sloan Foundation, the Participating Institutions, the National Science Foundation, the U.S. Department of Energy, the National Aeronautics and Space Administration, the Japanese Monbukagakusho, the Max Planck Society, and the Higher Education Funding Council for England. The SDSS Web Site is http://www.sdss.org/ [18].

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matter/

URLs in this post:

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[2] hlin@fnal.gov: **mailto:hlin@fnal.gov**
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[4] Image: **http://newscenter.lbl.gov/wp-content/uploads/stripe-82-run-2583-camcol-4-field-158-detail.jpg**
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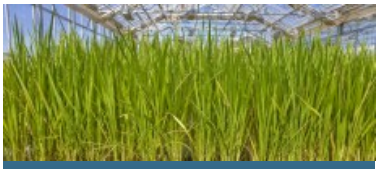
TURNING GRASS INTO GAS FOR LESS

Simulations Unlock Secrets of Cellulose Deconstruction

SEPTEMBER 30, 2011
Contact: Margie Wylie, mwylie@lbl.gov, +1 510 486 7421

Pull up to the pump these days and chances are your gas will be laced with ethanol, a biofuel made from corn. Corn-ethanol is relatively easy to make, but with growing populations and shrinking farmland, there will never be enough of the starchy food crop to both feed and fuel the world.



If researchers can unlock the sugars stored in plant cellulose, then crops like this switchgrass could be turned into biofuels, rather than using corn or other food crops.

That's why researchers are working on "grassoline," liquid biofuels made from hardy, high yielding, non-food crops, like switchgrass. But what makes these crops indigestible to humans also makes them challenging raw materials for biofuel production. The sugars needed to make biofuels are locked up tight in cellulose and researchers have yet to figure out an economical, scalable way to break them loose.

Recent computer simulations carried out at the National Energy Research Scientific Computing Center (NERSC) could help scientists do just that. The simulations show how two different solvents help unzip cellulose's structure, peeling off long strings of sugars. That information should help researchers engineer molecules that do the job better, cheaper, and on a larger scale, says Jhih-Wei Chu, a chemical and biomolecular engineering professor at the University of California Berkeley who ran the simulations at NERSC.

Computer simulations offer scientists an unparalleled view into processes that are practically unobservable. "If you try to measure cellulose degradation experimentally, it's just too messy: The signals overlap and it's impossible to isolate the individual forces and positions of molecules," he explains. "With simulations, we can calculate atom-by-atom, bond-by-bond exactly what is happening in a complex molecular system." Simulations also offer researchers the luxury of studying few billionths-of-a-second processes at human time scales, says Chu, whose is also a principal investigator with the **Energy Biosciences Institute** (EBI). EBI is a collaboration of the university, the U.S. Department of Energy's Lawrence Berkeley National Lab (which operates NERSC) and the energy company BP.

Cracking Cellulose

Cellulose is a polymer of the sugar glucose, the most important energy source for living things. Plants make glucose from sunlight, water and carbon dioxide through the process of photosynthesis. They link glucose molecules together with oxygen, forming long chains. Then the chains are aligned into sheets that are bound together with hydrogen bonds to form microfibrils of cellulose.

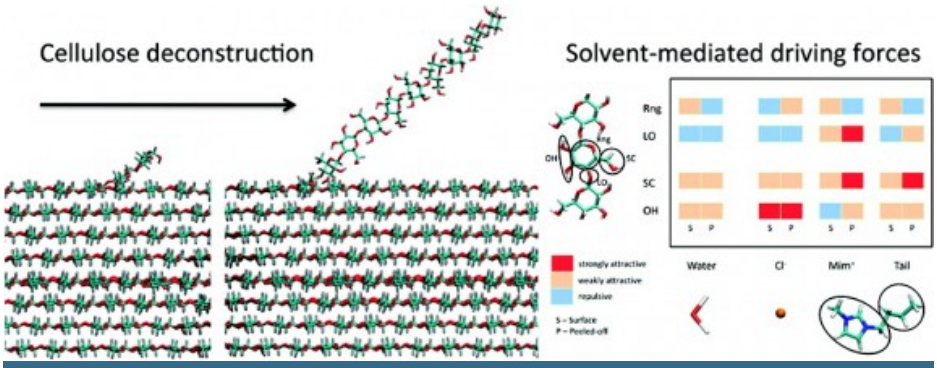
Humans now want to take that same building material and convert it back into energy. The problem is that cellulose is very tough stuff. "Plants have evolved to synthesize cellulose to resist breakdown," Chu says.

Still, cellulose isn't impervious to degradation. Toss an old cotton rag (about 90 percent cellulose) into your garden, and it will eventually degrade like other plant material, but it can take months or years. Scientists and engineers who work with biofuels use a variety of methods to help speed the process along, including steam, pressure, enzymes and solvents.

Chu simulated two aspects of celulose decomposition: solvent effects and enzyme actions.

Solvent Effects

In his first simulation study, Chu explored how liquid salts (ionic liquids, in scientific parlance) dissolve crystalline cellulose. Sodium chloride, common table salt, has a very compact crystalline structure so doesn't turn liquid until it reaches 800 degrees Centigrade. To get a salt that's liquid at much lower temperatures, the sodium cation (the positively charged ion) is replaced with a bulkier organic cation.



On the left, a strand of cellulose is peels off from the crystalline structure. On the right, the table documents the attractive forces between various components of cellulose and the ionic liquid. Select to enlarge. (Image courtesy Jhih-Wei Chu, UC Berkeley)

For his simulations, Chu used 1-butyl-3-methylimidazolium chloride (BmimCl). “We know this ionic liquid will dissolvecellulose, but we are really not sure why,” says Chu. “Along with my co-authors, I wanted to understand how the molecular forces provided by ionic liquids help deconstruct crystalline cellulose. That knowledge could allow us to design better solvents and engineering processes.”

In the lab there are many ionic liquids to choose from. That’s the good news. The bad news is that there are so many ionic liquids to choose from, that it is impractical for researchers to experiment with all possible candidates in a trial-and-error fashion. “If there are N cations and N anions to choose from, then there can be up to N^2 possible ionic liquids. That’s a lot to sort through,” says Chu. “To rationally design solvents for cellulose, you have to know what properties you are after, and how the ionic liquid interacts with cellulose. Therefore, a powerful ‘microscope’ with the ability to resolve molecular structures and also sense their interaction forces is needed. That is where computer simulation comes in.”

His simulation model, which contains approximately 100,000 clusters of atoms, required around one million CPU hours split between the Hopper system (a Cray XE6 supercomputer) and Carver (an IBM iDataplex cluster) to produce a few tens of billionths of a second of action. “The range of systems at NERSC is great for our work,” says Chu. “We run these enormous calculations on Hopper, but for some theory, the amount of memory per node is more important than the number of cores you can run at once and that’s where Carver comes in.”

Chu’s model breaks down the cellulose polymer into four different sections — the hexagonal ring (Rng), the linker oxygen (LO), the side chain (SC) and the hydroxol groups (OH). In turn, the interactions of these groups were tested against water, the anion (Cl-), the charged portion of the cation (Mim+) and the neutral tail portion of the cation (Tail). A table (above) summarizes the interactions between all these groups for a strand of cellulose before and after the solvent peels it off.

If the various components of cellulose are more attracted to each other than to the solvent, cellulose won’t dissolve. This is the case with water, a poor solvent for cellulose.

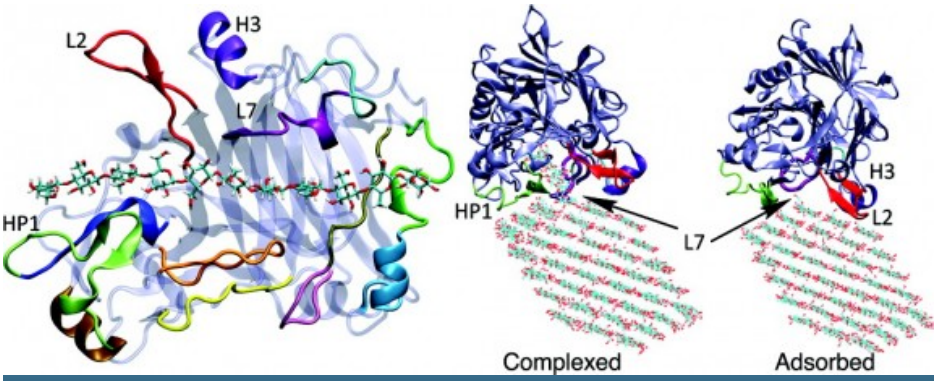
However, in BmimCl the components of cellulose are more attracted to the components of the ionic liquid than they are to each other and the cellulose dissolves.

Chu and collaborators found that this solvent is very versatile, attacking a variety of bonds in the crystalline structure. “The Cl anions have strong attraction to hydroxol groups and weak attraction to side chains and sugar rings, while the cations have strong attractions to side chains and linker oxygens,” says Chu. “This versatility can potentially be employed as the basis for molecular design and engineering.”

In a second simulation study, Chu and colleagues examined the workings of a small portion of a much more complex system, a cellulase enzyme.

Enigmatic Enzymes

Evolution has endowed some organisms with cellulases, enzymes that can break down cellulose. Cow and termites digest cellulose, although they rely on cellulases of symbiotic bacteria living in the acidic environment of their digestive tracts. Humans can’t digest the cellulose in our food. We call it fiber.



A strand of cellulose passes through the active site of the Trichoderma reesei cellulase enzyme. One

portion of the enzyme, marked L7, acts like an ice cream scoop, physically peeling up a fibril and lifting it into the active site for digestion. Select to enlarge. (Image courtesy Jhih-Wei Chu, UC Berkeley)

One of the best sources of cellulases is the fungus *Trichoderma reesei.* During WWII in the South Pacific, the U.S. Army discovered that its canvas tents were dissolving in the heat and humidity. Army researchers isolated the fungus feeding on their tents, and it has been an important source of cellulases ever since.

Like ionic liquids, researchers have been using cellulases to degrade cellulose without entirely understanding how they work.

In a recent simulation Chu and collaborators found that a portion of a *T. reesei* cellulase acts something like an ice cream scoop, physically peeling up microfibrils of cellulose and lifting them into the maw of the enzyme for digestion. The simulation hints at ways industrial enzymes already in use might be improved, says Chu.

“Computer simulation of molecular dynamics and interactions really is like a huge crowd shot in a movie. As the director, there is so much detail at your disposal that you can lose sight of the plot. Knowing where to zoom in requires some judgment and intuition,” says Chu. “I think we were able to distill the essential plot elements that we hope biofuel researchers will be able to develop further.”

“**Dissecting Force Interactions in Cellulose Deconstruction Reveals the Required Solvent Versatility for Overcoming Biomass Recalcitrance**,” appeared in the *Journal of the American Chemical Society* on July 28, 2011.

“**Protein Allostery at the Solid-Liquid Interface: Endoglucanase Attachment to Cellulose Affects Glucan Clenching in the Binding Cleft**,” appeared in the *Journal of the American Chemical Society* on August 30, 2011.

About NERSC and Berkeley Lab

The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy's Office of Science. Located at Lawrence Berkeley National Laboratory, the NERSC Center serves more than 4,000 scientists at national laboratories and universities researching a wide range of problems in combustion, climate modeling, fusion energy, materials science, physics, chemistry, computational biology, and other disciplines. **Berkeley Lab** is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the U.S. DOE Office of Science. For more information about computing sciences at Berkeley Lab, please visit **www.lbl.gov/cs**.

More Information

»**Learn about the Chu Research Group**

»**Learn about the Energy Biosciences Institute**

»**Visit Jhih-Wei Chu's Faculty webpage**

»**Read the UC Berkeley College of Chemistry Article**

A Better Way to ID Extreme Weather Events in Climate Models

Posted By dankrotz On December 6, 2011 @ 2:36 pm In Feature Stories | Comments Disabled

You'd think that spotting a category 5 hurricane would never be difficult. But when the hurricane is in a global climate model that spans several decades, it becomes a fleeting wisp among mountains of data.

That's a problem. As scientists develop ever-more sophisticated computer models to predict the effects of climate change, one of the things they'll look for are changes in the frequency of extreme weather events such as hurricanes and heavy precipitation. The more data generated by models, however, the more difficult it is to quantify these rare but potent events.

What's needed is an automated way to quickly comb through a climate simulation's huge dataset and tally the weather events that spell big trouble. A team of researchers that includes scientists from Lawrence Berkeley National Laboratory (Berkeley Lab) are developing techniques to do just that.

"We're using state-of-the-art methods in data mining and high performance computing to locate and quantify extreme weather phenomena in the very large datasets generated by today's climate models," says Prabhat, a scientific visualization expert in Berkeley Lab's Computational Research Division. "We want to help answer the question: How will climate change impact the frequency of extreme weather?"

The research is led by fellow Berkeley Lab scientists Wes Bethel, Bill Collins and Michael Wehner, and includes scientists from Oak Ridge National Laboratory, Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and the University of California at Berkeley. Prabhat is presenting examples of their work Thursday morning (Dec. 8) at the annual meeting of the American Geophysical Union in San Francisco (8:30 a.m., room 102).

A one-year portion of a recent high-resolution atmospheric simulation that was conducted on NERSC.

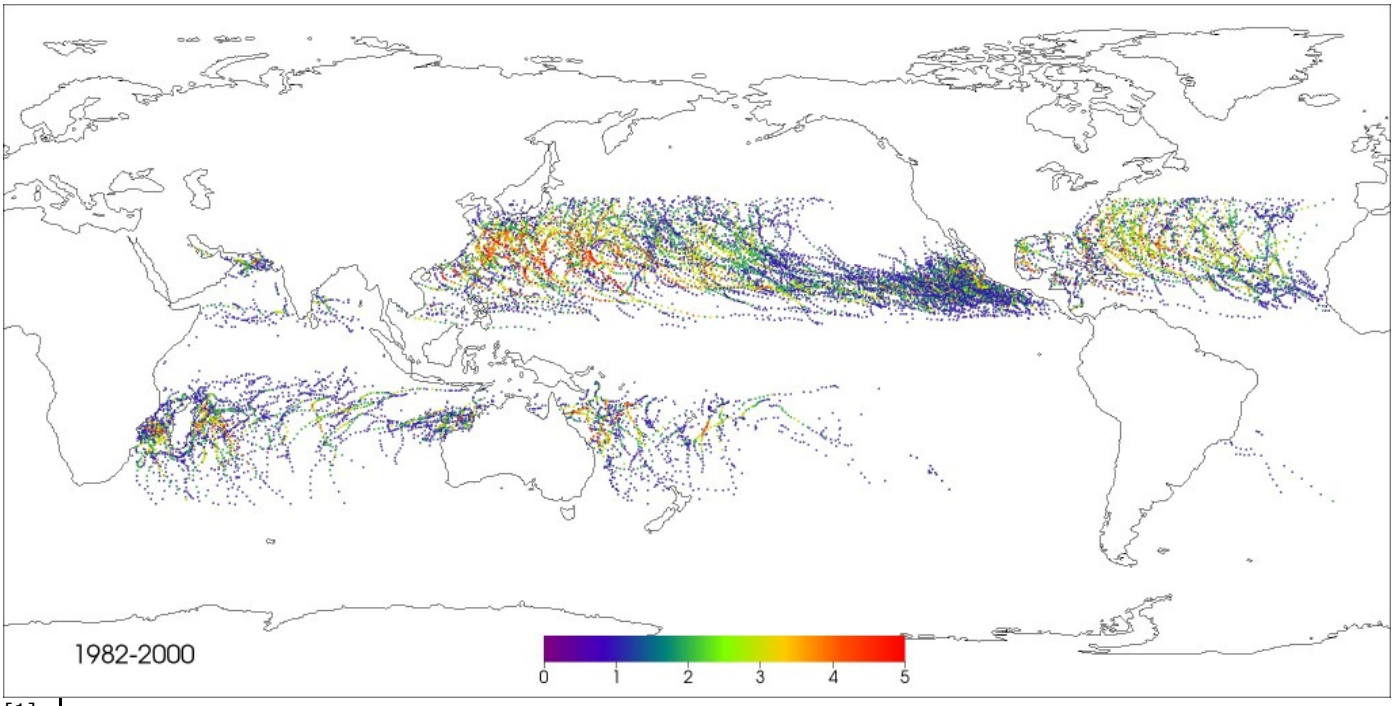
In one example, the scientists began with a recent run of the Community Atmospheric Model (CAM5), which is the latest in a series of global atmosphere models developed primarily at the National Center for Atmospheric Research. The high-resolution simulation spanned from 1979 to 2005 and is being used to demonstrate how well the model reproduces observed tropical cyclones. It was conducted on Hopper, a Cray XE6 supercomputer at the National Energy Research Scientific Computing Center (NERSC), which is located at Berkeley Lab.

The 27-year simulation generated 100 terabytes of data. In comparison, as of September 2011, the Library of Congress has collected about 254 terabytes of data.

To detect the hurricanes and cyclones in this simulation, the scientists used code from a model that tracks the intensity of hurricanes and cyclones, and adapted it to run in parallel on large datasets. In this case, the technique churned through the CAM5 simulation in two hours using 7000 cores at NERSC. It successfully quantified the hurricanes that appear in the simulation. The same process would have taken 583 days on a conventional desktop computer.

In another example, the scientists developed a pattern-detection algorithm that sifts through large datasets for a weather phenomenon called an atmospheric river. These are narrow corridors of water vapor that occur at mid-latitudes around the world. People who live on the Pacific coast of North America may know the phenomenon as a pineapple express, which channels moisture from the Hawaiian Islands to the west coast. These powerful storms can bring torrential rain, floods, and damaging wind.

The scientists used techniques from image processing and topological analysis to extract the telltale features of atmospheric rivers from satellite images and climate models. They then implemented these techniques in a massively parallel fashion on a supercomputer platform to automatically detect

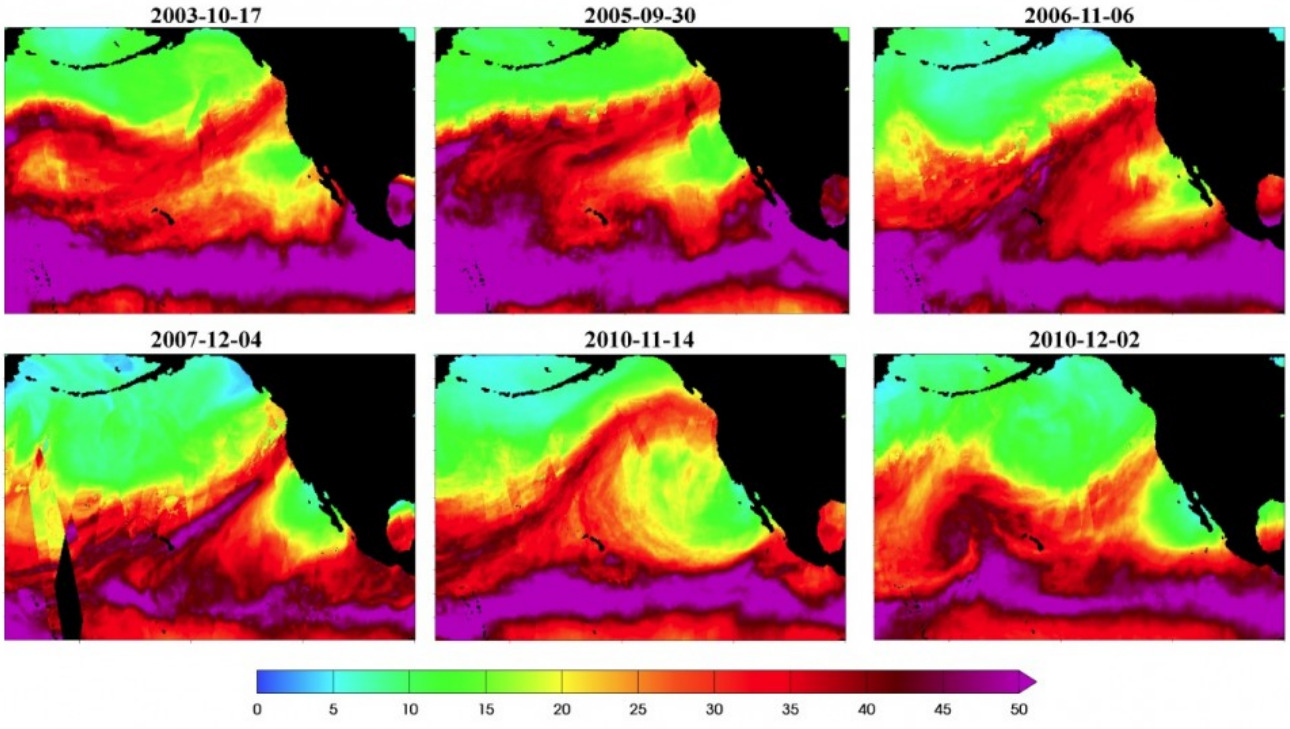


[1]

Category 1 through 5 hurricanes and cyclones detected in the CAM5 simulation

these events in large datasets.

They applied this software to satellite images from 2002 to 2010 and atmospheric modeling data from 1979 to 1993, representing 640 gigabytes of data in all. The software processed this data in about three seconds using 8500 cores on the NERSC Hopper system, and detected 92 percent of the atmospheric rivers that made landfall. The same process would have taken several hours on a conventional desktop computer.



[2]

Some typical atmospheric river events detected by the new method from the observational dataset. Shown

is total column integrated precipitable water in millimeters. Note that data irregularities in the satellite measurements (such as the abrupt discontinuities in the 2007-12-04 event) do not have an adverse effect on the detection procedure.

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This research was supported by the U.S. Department of Energy's Office of Science. NERSC is supported by the Department of Energy's Office of Science.

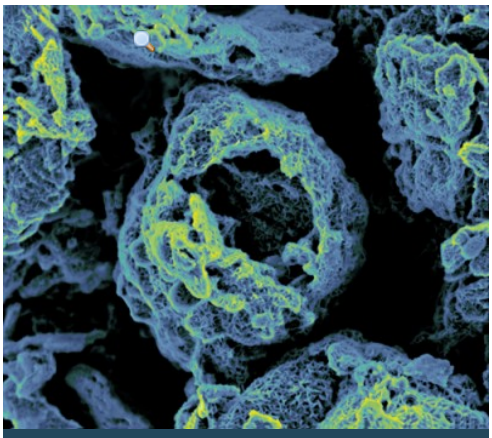
Lawrence Berkeley National Laboratory addresses the world's most urgent scientific challenges by advancing sustainable energy, protecting human health, creating new materials, and revealing the origin and fate of the universe. Founded in 1931, Berkeley Lab's scientific expertise has been recognized with 13 Nobel prizes. The University of California manages Berkeley Lab for the U.S. Department of Energy's Office of Science. For more, visit www.lbl.gov [3].

BUBBLES HELP BREAK ENERGY STORAGE RECORD FOR LITHIUM AIR-BATTERIES

Foam-base graphene keeps oxygen flowing in batteries that holds promise for electric vehicles

JANUARY 25, 2012 | Tags: Energy Technologies, Hopper, Materials Science
Linda Vu, lvu@lbl.gov, +1 510 495 2402

One of the biggest weaknesses of today's electric vehicles (EV) is battery life—most cars can only go about 100-200 miles between charges. But researchers hope that a new type of battery, called the lithium-air battery, will one day lead to a cost-effective, long-range EV that could travel up to 300 miles or more between charges.



Using a new approach, the team built a graphene membrane for use in lithium-air batteries, which could, one day, replace conventional batteries in electric vehicles. Resembling coral, this porous graphene material could replace the traditional smooth graphene sheets in lithium-air batteries, which become clogged with tiny particles during use.

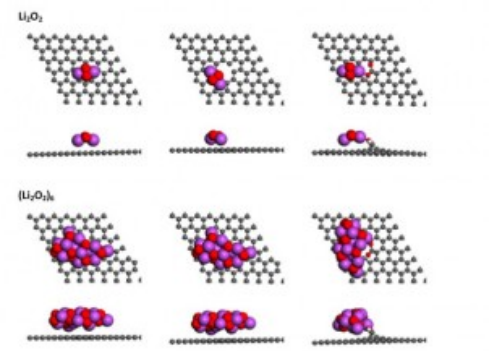
Using supercomputers at the National Energy Research Scientific Computing Center (NERSC) and microscopy, a team of researchers from the Pacific Northwest National Laboratory (PNNL) and Princeton University recently built a novel graphene membrane that could produce a lithium-air battery with the highest-energy capacity to date.

Composed of an atom-thick sheet of carbon, graphene is both the strongest and most conductive material ever measured. The new membrane is built from graphene formed around bubbles, and resembles broken eggshells. The researchers believe that this black, porous material could replace traditional smooth graphene sheets in lithium air batteries, which become clogged with tiny particles during use. Because the material does not rely on platinum or other precious metals, the researchers say that its potential cost and environmental impact are significantly less than current technology.

"This hierarchical structure of self-assembled graphene sheets is an ideal design not only for lithium-air batteries but also for many other potential energy applications," said Dr. Jie Xiao, the materials scientist at PNNL who led the study.

The researchers built the material by combining a binding agent with graphene, and similar to the way soap disperses grease in dishwater, the binding agent dispersed graphene in the solution. The graphene and binder were then added to water and mixed using a process that created bubbles in the solution. The graphene and binder then formed and hardened around the bubbles. When these bubbles popped, hollow spheres of graphene, about 3 to 4 microns in diameter (10 times smaller than human hair), were left behind.

Once the membrane was created, team members used both modeling and electron microscopy to analyze the graphene structures and their performance. They studied the particles using electron microscopy at the Environmental Molecular Sciences Laboratory, then performed density functional theory calculations on NERSC's Franklin and Hopper systems to further investigate behaviors that they noticed in the microscopy experiments. These simulations helped them figure out how to manipulate the material.



Properties of the new graphene membrane simulated on NERSC systems. Carbon atoms are represented in gray, lithium atoms are purple and oxygen atoms are red.. In each structure, the top and side views are shown in the upper and lower panel, respectively. (Image by Donghai Mei, PNNL)

Ultimately, the researchers found that the black porous structures store more than 15,000 milliamp hours per gram of graphene, making it far denser in energy capacity than other materials. The NERSC simulations were performed by PNNL scientist, Donghai Mei.

"Many catalysts are studied now for this technology. In our process we chose not to use precious metal," said Dr. Ji-Guang Zhang, the group leader in PNNL's lithium-air battery research. "This will greatly reduce production costs and increase the adoptability."

Although the battery is achieving the highest level of energy capacity in an oxygen-only environment, when operated in ambient air, the capacity drops because water vapor in the air fouls the lithium metal in the batteries. The PNNL team is working to develop a membrane to block the water and still allow the necessary oxygen to flow.

"We also want to make the battery rechargeable," said Zhang. "Right now, it is not. It is not fully rechargeable. We are working on a new electrolyte and a new catalyst so that the battery can be recharged multiple times, potentially for battery backup applications that require high energy densities."

This story was adapted from a PNNL research highlight. The paper was published in ACS Chemical & Engineering News.

About NERSC and Berkeley Lab

The National Energy Research Scientific Computing Center (NERSC) is the primary high-performance computing facility for scientific research sponsored by the U.S. Department of Energy's Office of Science. Located at Lawrence Berkeley National Laboratory, the NERSC Center serves more than 4,000 scientists at national laboratories and universities researching a wide range of problems in combustion, climate modeling, fusion energy, materials science, physics, chemistry, computational biology, and other disciplines. **Berkeley Lab** is a U.S. Department of Energy national laboratory located in Berkeley, California. It conducts unclassified scientific research and is managed by the University of California for the U.S. DOE Office of Science. For more information about computing sciences at Berkeley Lab, please visit **www.lbl.gov/cs**.