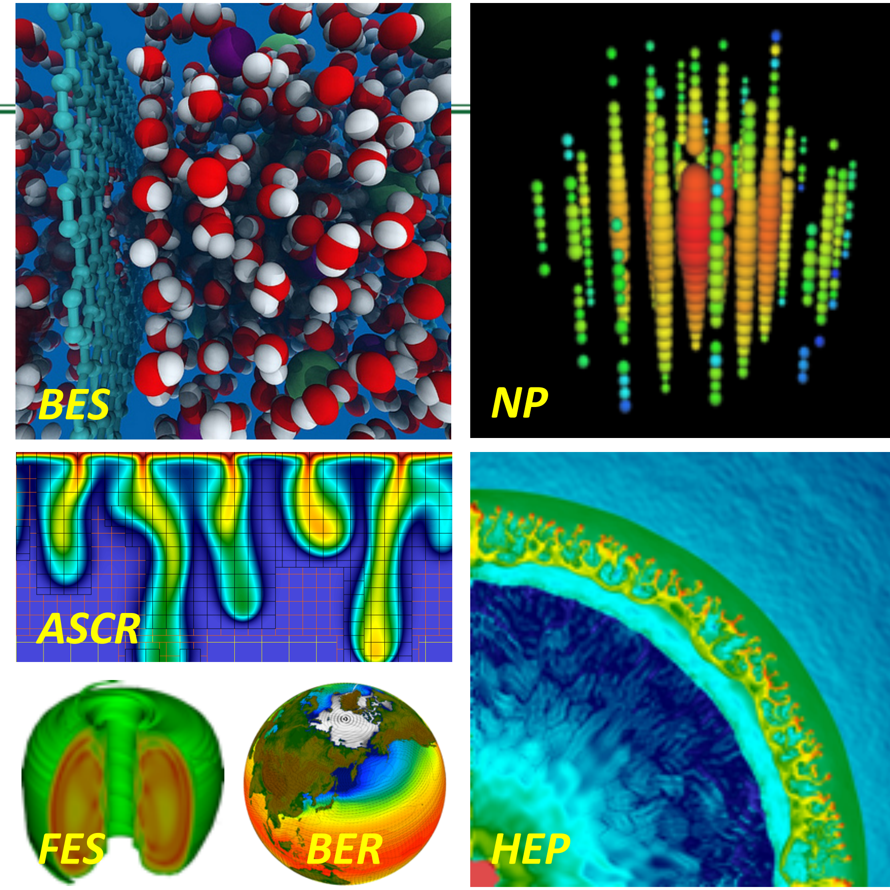
# NERSC Science Highlights

# July 2016



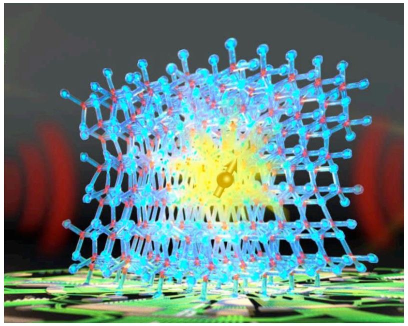

NERSC

BERKELEY LAB
Lawrence Berkeley National Laboratory

U.S. DEPARTMENT OF ENERGY | Office of Science

# Science Highlights July 2016

NERSC



## Materials Science

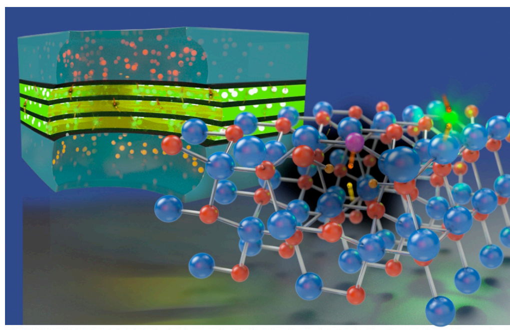
Calculations confirm a less expensive material for making quantum bits. **(Govoni/Galli, Univ. of Chicago, *Nature Scientific Reports*)**

## Applied Math

A new mathematical framework allows researchers to capture fluid dynamics at unprecedented detail. **(Saye, LBNL, *Science Advances*)**

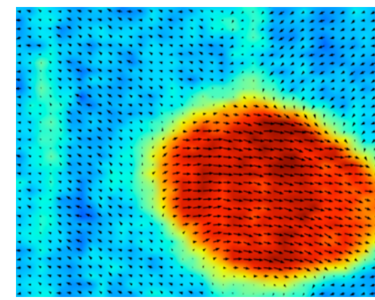
## Materials Science

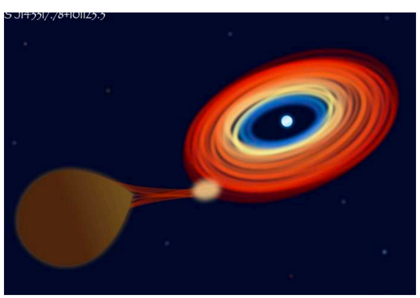
Simulations point to more efficient light emitting diodes. **(Dreyer et al.,UC Santa Brabara, *Applied Physics Letters***



## Energy/Materials

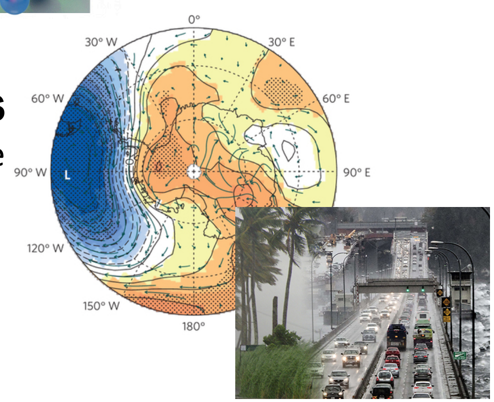
Multiscale simulations run on Edison explain behavior of ferroelectric materials. **(Rappe, Univ. of Pennsylvania, *Nature*)**





## High Energy Physics

Model confirms existence of an irradiated brown-dwarf companion to an accreting white dwarf. **(Baron, U. Oklahoma, *Nature*)**




## Climate Research

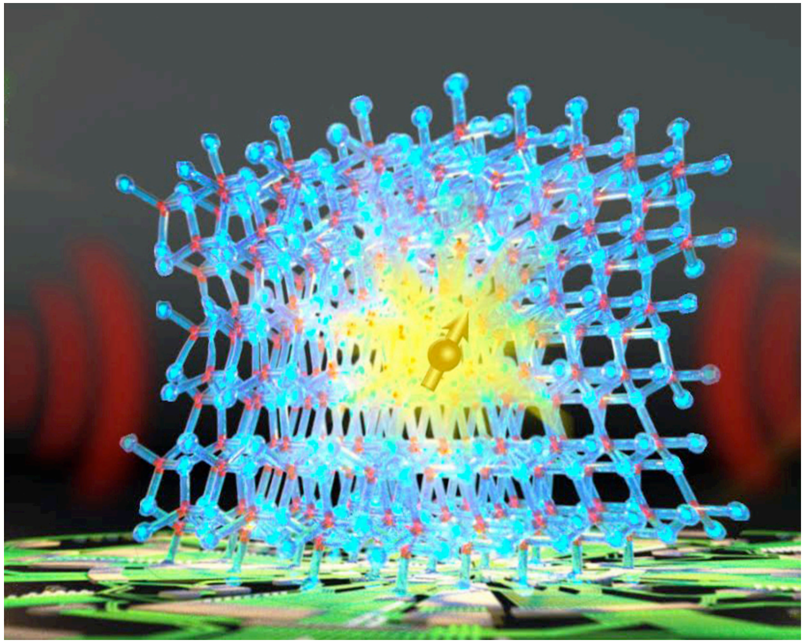
Simulations show why Antarctic sea ice is expanding. **(Meehl, NCAR, *Nature Geoscience)***

Understanding interactions between climate and regional weather. **(Hagos, PNNL, *Journal of Climate*)**

# Better Materials for Quantum Computing

## Scientific Achievement

One of the leading methods for creating quantum bits (qubits) involves exploiting the structural atomic defects in diamond. However, using diamond is both technically challenging and expensive. Now researchers from the University of Chicago and Argonne National Laboratory have found a way to engineer an analogue defect in aluminum nitride, which could reduce the cost of manufacturing quantum computers.



***This graphic illustrates an engineered nitrogen vacancy in aluminum nitride***

## Significance and Impact

Quantum computers have potential to break common cryptography techniques, search huge datasets and simulate quantum systems in a fraction of the time it takes today's computers. But engineers first need to be able to control the properties of qubits.

## Research Details

- Using NERSC's Edison supercomputer, the researchers found that by applying strain to aluminum nitride, structural defects can be created in the material that may be harnessed as qubits similar to those seen in diamond.
- Their calculations were performed using different levels of theory and the WEST code, developed at the University of Chicago, which allowed them to accurately predict the position of the defect levels in the band-gap of semiconductors.

*Seo, Govoni, Galli, Nature Scientific Reports, Vol. 6, Article No. 20803, Feb. 16, 2016*

# Interactions Between Climate and Regional Weather

## Scientific Achievement

Pacific Northwest National Laboratory researchers are using field data and NERSC supercomputers to better model how the Madden-Julian Oscillation (MJO) – a moving disturbance of clouds, rainfall, winds and pressure –operates and gain new understanding of its interaction with regional weather systems around the world.

## Significance and Impact

Better understanding of the MJO is vital. Its unpredictability makes it harder for weather forecasting many regions around the world including Western U.S., Australia and South Asia. Despite decades of work, however, simulating the MJO in climate models and understanding the instabilities that drive it remain a significant challenge.

***From Calcutta, India, to Seattle, Wash. and beyond, the MJO can bring storms and plenty of rain in wet years.***

## Research Details

- Using NERSC's Edison supercomputer and data gathered during a field campaign over the Indian Ocean, the researchers identified the processes that are responsible for too much precipitation in the models, especially during the low-rainfall period of the MJO signal.
- The simulations, which used 2,400 cores and about 250,000 computer hours, found that the mismatches are related to the fact that most models get the relationship between environmental moisture and precipitation wrong, producing more precipitation than is observed for the same moisture content in the environment.

S. Hagos, et al, *Journal of Climate*, Vol. 29, No. 3, February 2016, 1091-1107

# Design and Discovery of New Ferroelectric Materials

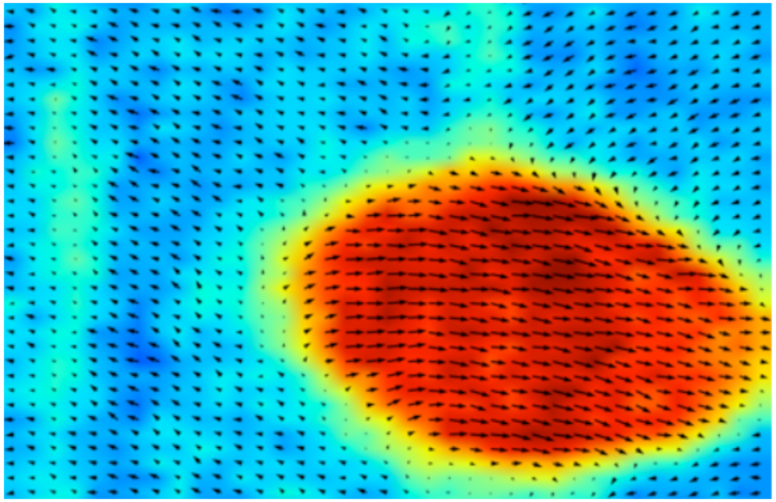
## Scientific Achievement

Chemists from the University of Pennsylvania demonstrated a multi-scale simulation, run at NERSC, of lead titanate oxide that provides new understanding about what it takes for polarization within ferroelectric materials to switch.

## Significance and Impact

Ferroelectric materials are useful because their magnetic polarization makes them rotate to align with magnetic fields. They are crucial “smart materials” for sensors, such as ultrasound machines and probe-based microscopes.

Despite proliferation in commercial applications, however, there are many gaps in the theoretical principles that explain the behavior of ferroelectric materials. This new mathematical model is expected to aid efforts to find and design new ferroelectric materials.



***Simulations run at NERSC demonstrated that thermal fluctuations in ferroelectric materials are responsible for the first nuclei from which changes in polarization spread.***

## Research Details

- The ferroelectric material simulated on NERSC’s Edison system features titanium ions inside six-pointed octahedral “cages” of oxygen ions. The polarization of a given domain is determined by which points of the cages the titanium ions move toward.
- This study is the first to show that math models calibrated to quantum mechanics can accurately relate the strength of the electric field to the speed at which domain walls move.

S. Liu, I. Grinberg, A.M. Rappe, *Nature* 534, 360–363, , June 16, 2016

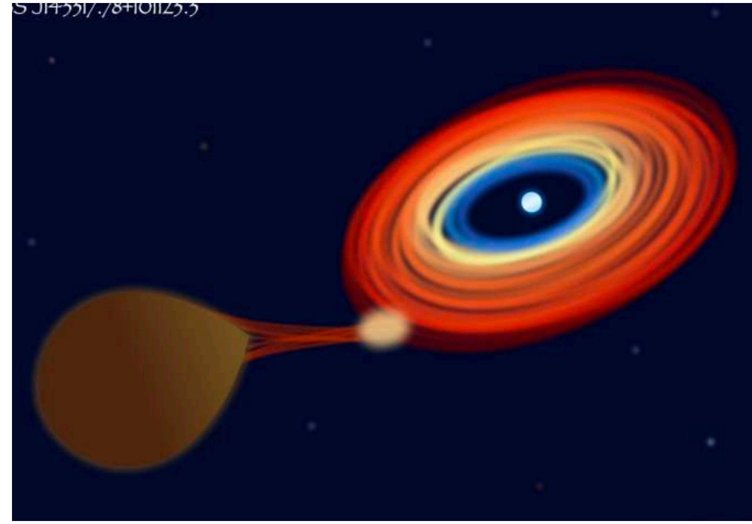
# Brown-Dwarf Companion to Accreting White Dwarf

## Scientific Achievement

In a recent Nature paper an international research team used spectroscopic observations and theoretical predictions to confirm the existence of an irradiated brown-dwarf companion to an accreting white dwarf.

## Significance and Impact

Astronomers want to better understand how planetary and star systems beyond our own were formed, live, and die. One of the more interesting situations occurs when a compact "white dwarf" star accretes material from a nearby "brown dwarf," an object that is too small to be a star, yet too large to be called a planet. To date, only a single brown-dwarf donor to an accreting white dwarf has been detected, and no empirical information is available regarding the effect of irradiation on the atmosphere of the donor.



***This image shows the white dwarf (right) stripping mass from the brown dwarf. Credit: Rene Breton, University of Manchester.***

## Research Details

- This work employed PHOENIX, a general-purpose stellar and planetary atmosphere code that can calculate atmospheres and spectra of stars, including white dwarfs and brown dwarfs; and ICARUS, a binary light-curve synthesis code.
- The computations, run NERSC's Edison supercomputer, allowed the team to model and characterize the signature of the brown dwarf atmosphere.

J.V. Hernandez Santisteban, et al, *Nature* 533, May 2016, 366–368

# How Climate Fluctuations Influence Sea Ice Expansion

## Scientific Achievement

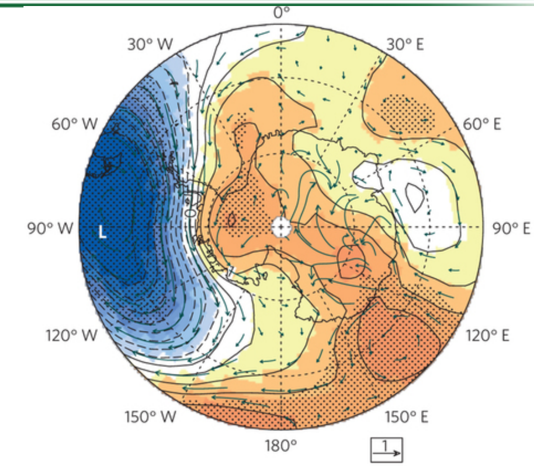
Observations indicate that the Antarctic sea ice been expanding since 2000, while the average findings of all climate models shows a decline. A new study, led by the National Center for Atmospheric Research (NCAR), found that the expansion can be explained by natural climate fluctuation.

## Significance and Impact

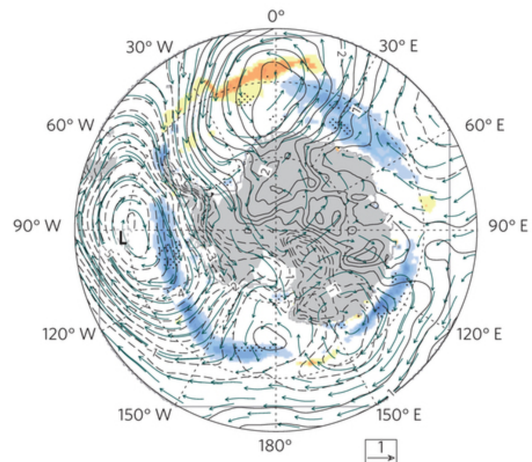
Surface wind changes that have expanded Antarctic sea ice mainly driven by sea surface temperature and precipitation anomalies from the naturally occurring Interdecadal Pacific Oscillation (IPO) in the equatorial eastern Pacific, and climate models can simulate these processes.

## Research Details

- By comparing physical observations with climate model simulations run at NERSC, NCAR researchers were able to demonstrate a direct connection between Antarctic sea-ice expansion and the IPO.
- The study offers evidence that the negative phase of the IPO, which is characterized by cooler-than-average sea surface temps in the tropical eastern Pacific, has created favorable conditions for the sea ice growth since 2000.




***An idealized climate model with negative precipitation and convective heating anomalies in the Pacific makes a direct connection between negative IP, deeper Amundsen Sea Low, northward surface wind anomalies and expanding Antarctic sea ice.***




***Observed expanding Antarctic sea ice (blue shading) shows that since the 2000 IPO transition to negative are connected to a deeper Amundsen Sea Low ("L").***

G.A. Meehl, et al,
*Nature Geoscience*,
July 4, 2016, doi:
10.1038/ngeo2751

# Efficiency-Limiting Defects in LEDs

## Scientific Achievement

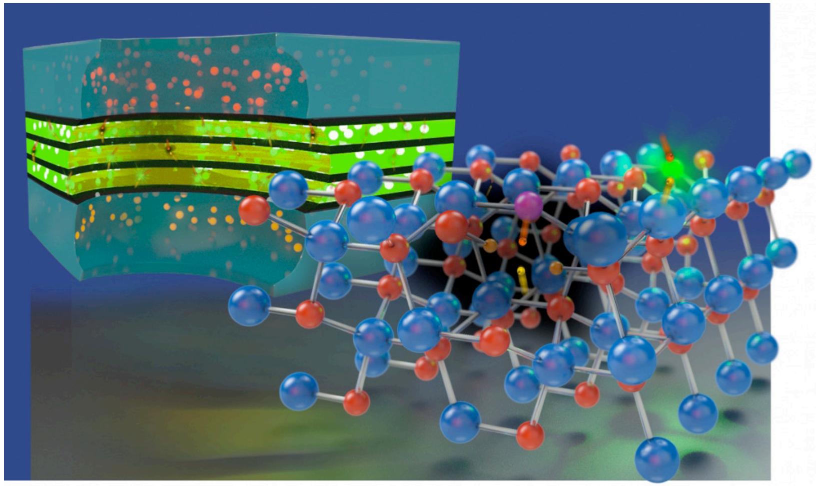
Using first-principles methods based on density functional theory, UC Santa Barbara (UCSB) researchers have identified materials defects that act as sites for nonradiative recombination, which can explain the observed reduction in efficiency of nitride-based light emitting diodes (LEDs).

## Significance and Impact

The work points the way toward fabrication of more efficient electronic and optoelectronic devices, a central goal for solid-state lighting and other devices.

## Research Details

- This research, which used 500,000 hours on NERSC supercomputers, addresses a problem that has been around for nearly 70 years.
- Others have reported experimental observations of nonradiative recombination (also known as Shockley-Read-Hall recombination) and have attempted to model it using empirical modeling, but were unsuccessful. This work is the first time a computational model has been able to reliably predict what specific defects are doing.



***A conceptual illustration of how defects in a crystal lattice might contribute to nonradiative recombination of electrons and holes in LEDs.***

C. Dreyer, A. Alkauskas, J. Lyons, J. Speck, C. Van de Walle, *Applied Physics Letters*, 108, April 2016, 141101

PI: C. Van de Walle (Univ. of California, Santa Barbara)

# ‘New Math’ Captures Fluid Interface Dynamics in Unprecedented Detail

## Scientific Achievement

A new mathematical framework developed at Berkeley Lab and tested on NERSC supercomputers sheds new light on how fast a fluid is moving in its environment, how much pressure it is under and what forces it exerts on its surroundings.

## Significance and Impact

Gas bubbles, thin films, flowing blood and ocean can all be mathematically modeled as interface dynamics coupled to Navier-Stokes equations, which predict how fluids flow. But computational methods for solving these equations have not been able to accurately resolve the often-intricate fluid dynamics taking place next to moving boundaries and surfaces. The new algorithms accurately resolve the intricate structures near the surfaces attached to the fluid motion.

***This computer rendering illustrates the results of a simulation studying a ripple phenomenon in a water jet caused by surface tension.***

## Research Details

- Berkeley Lab researchers developed a new mathematical framework that allows researchers to capture fluid dynamics at unprecedented detail. The work could be used in a range of applications, such as optimizing the shape of a propeller blade and the ejection of ink droplets in printers.
- Many of the computations for this research were run on NERSC’s Edison supercomputer. The development of these algorithms requires extensive convergence studies and simulation in two and three dimensions by performing a substantial number of simulations, each one using hundreds-to-thousands of cores.

R. Saye, *Science Advances*, Vol. 2, No. 6, June 3, 2016

NERSC

National Energy Research Scientific Computing Center