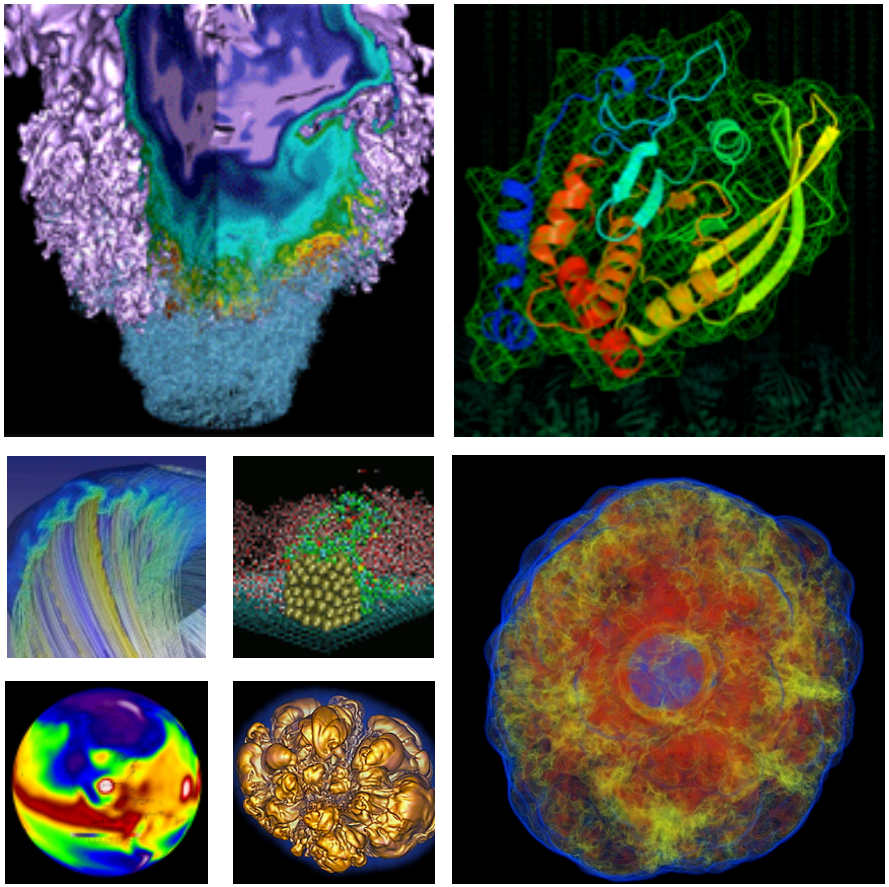
NERSC Science Highlights



Selected User Accomplishments

July 2013

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

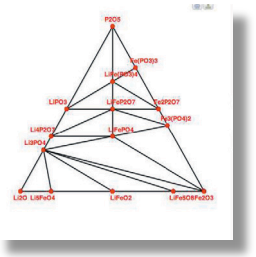
NERSC User Science Highlights

Nuclear Physics

NERSC resources aid worldwide collaboration that discovers neutrinos of unprecedented energy
(L. Gerhardt, LBNL)

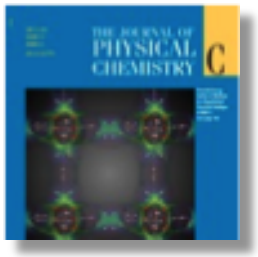
Materials

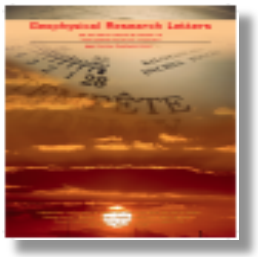
NERSC collaboration yields software that is a key enabler in the high-throughput computational materials science initiative
(S. Ong, MIT)



Materials

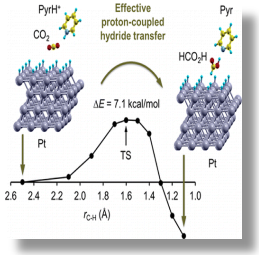
Model is able to predict which of a million or so potential materials might be best for carbon capture
(B. Smit, LBNL)





Climate

Independent confirmation of global land warming without the use of land thermometers
(G. Compo, U. Colorado)

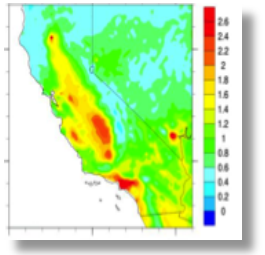


Chemistry

Study helps explain an important reaction that converts CO_2 to organic chemicals
(V. Batista, Yale)

Climate

NERSC simulations contribute to a study finding that emission regulations reduced soot and climate change impact in California
W. Collins (LBNL)



IceCube Finds Neutrinos Invading from Another Galaxy

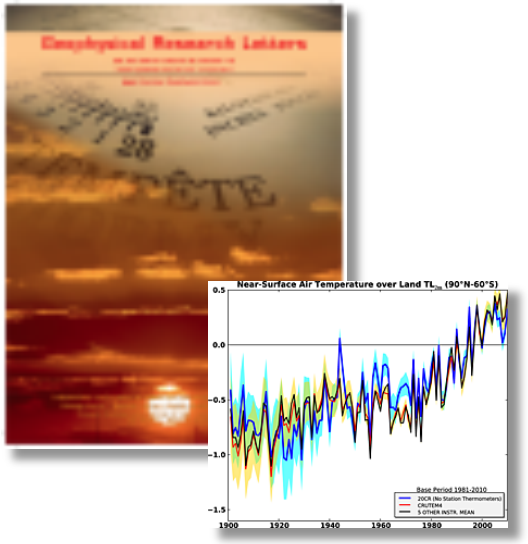
- Neutrinos are unique astrophysical messengers that open a new window on the universe.
- The IceCube neutrino telescope is a $242M device made of 5,160 sensors buried 1.5 km beneath the South Pole.
- IceCube detected two events with energies of about 10^{15} eV (Peta-ElectronVolts - roughly equivalent to the energies reached at the LHC).
- Collaboration of 39 universities and labs relied on NERSC PDSF and Carver for data analysis and simulation.
- Experimental and simulation data sets archived on NERSC HPSS

On the Cover: Schematic of one of the two PeV-energy neutrino events detected by the IceCube detector. Each sphere represents a detector sensor. Sphere size is a measure of detector response. Colors represent arrival times (red, early; blue, late). These two events could be the first ever hints of neutrinos from astrophysical sources.

Phys. Rev. Lett. 111 (2013) 021103

First Independent Confirmation of Global Land Warming

- **Goal: Check the accuracy of land-based temperature measurements that show a warming trend over the last 100 years**
  - To address a climate change research concern that older data aren't accurate
- **Accomplishment: A computer model that infers temperature from alternate sources**
- **Significance: Confidence in estimates of human-caused climate change is limited by known issues with older thermometer-based air temperature observations. This independent model shows that the measured temperature record is reliable, demonstrating the robustness of conclusions regarding global warming reached by IPCC and others.**



On the Cover: Confirmation of land warming that used data from the 20th Century Reanalysis project instead of from land station measurements. Inset shows a comparison of measured and predicted average global temperatures for 1900 through 2010.

Geophys. Res Lett
pages 3170–3174, 28 June 2013

Mail-Order Metal Organic Frameworks

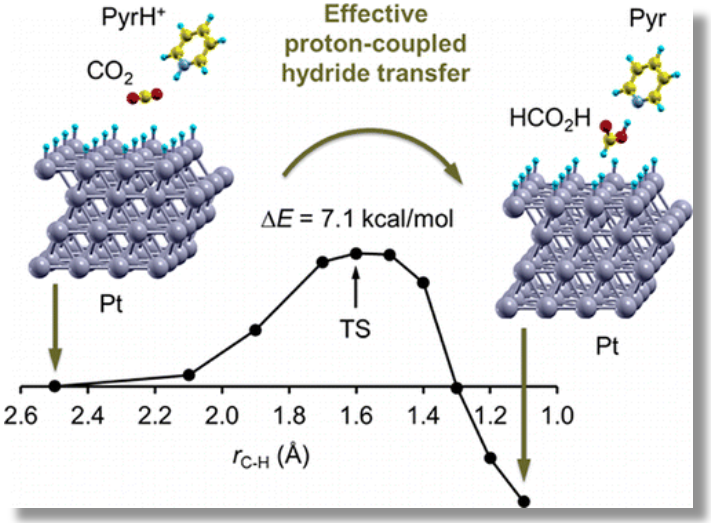
- **Accomplishment: development of an automated procedure for designing and evaluating hypothetical metal–organic frameworks (MOFs), a class of porous materials of interest in gas storage and separation applications.**
- **MOFs may be more efficient for capturing CO_2 emissions from coal power plants.**
- **The new model is able to predict which of the million or so potential MOFs might be best for carbon capture.**
  - Eliminates expensive, time-consuming lab work
- **Results are stored in a Carbon Capture Materials Database, accessible by researchers throughout the world**

On the Cover: Computed structures of Metal-Organic Frameworks that are highly porous materials of particular interest in gas storage and separation applications

Journal of Physical Chemistry C
June 13, 2013: Vol. 117, Iss. 23

Study Shows How a Greenhouse Gas Could be Converted to Fuel

- Researchers have used computation to explain how carbon dioxide can be converted to small organic molecules with little energy input.
- An important strategy for reducing global CO_2 emissions calls for capturing the greenhouse gas and converting it to fuels and chemicals.
- Although researchers working toward that goal demonstrated in 1992 such a reaction in the lab, a key outstanding scientific challenge was to explain the details of how the reaction took place.
- The reaction mechanism revealed through computation at NERSC is viewed as being particularly valuable for the design and development of new technologies that would generate fuels with a carbon-neutral footprint.



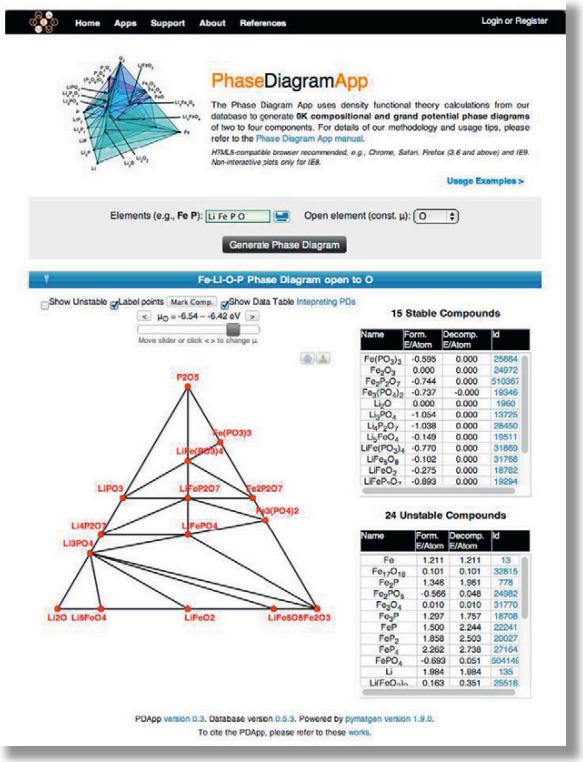
Results of electronic structure computations done at NERSC explaining the precise mechanism of a reaction in which CO_2 is converted to formic acid (HCO_2H, an important intermediate in chemical synthesis) using platinum (Pt)

J. Phys. Chem. Lett., 2013, 4 (5), pp 745–748

Chemical & Engineering News Volume 91 Issue 10 | p. 29 | March 11, 2013

NERSC Collaboration will Improve Materials Analysis

- **Accomplishment: A robust, open-source Python library for materials analysis has been developed and deployed at NERSC.**
- **Significance: Has already become a key enabler in high-throughput computational materials science efforts.**
- **Resulted from close collaboration between materials and computer science researchers and NERSC staff.**
- **Powers several of the *Materials Project*'s web applications and provides convenient tools to obtain useful materials data.**
- **Demonstrated how a recently synthesized lithium-ion battery material could be analyzed using a minimum of computing resources.**

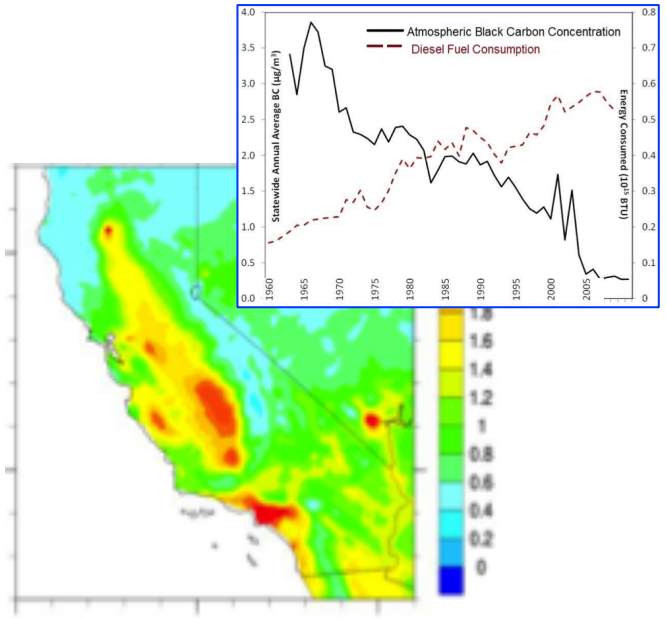


A view of the Phase Diagram Application from the pymatgen software package.

Computational Materials Science Vol 68 (2013) 314–319

Reduced Climate Change Impact in California from Emission Regulations

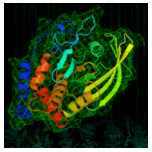
- Climate simulations carried out at NERSC played a key role in a report recently sponsored by the California Air Resources Board (CARB) examining Black Carbon and the Regional Climate of California.
- The report suggests that reductions in emissions of soot since the late 1980s, mostly from diesel engines as a result of air quality programs, have resulted in a measurable reduction of global warming pollutants in the atmosphere over California.
- The first-of-its-kind study estimated that reductions in black carbon as a result of clean air regulations were equivalent to reducing carbon dioxide emissions in California by 21 million metric tons annually – the same as taking some 4 million cars off California roads every year.



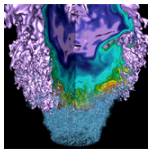
Lower Left: Atmospheric heating due to soot according to WRF simulation done at NERSC. Upper Right: atmospheric black carbon concentration (black) and Diesel fuel consumption from 1960 to 2012.

http://www.arb.ca.gov/research/single-project.php?row_id=64841

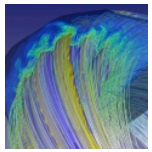
About the Title Slide Images



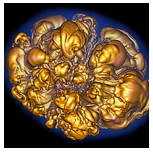
Snapshot from a simulation of a protein folding to its preferred shape, one of many such simulations done at NERSC as part of the Dynameomics Project (Valerie Daggett, U. Washington)



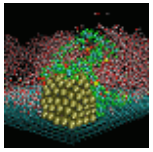
Detailed structure of a flame from a Low swirl burner combustion simulation. Image courtesy of John Bell, LBNL.



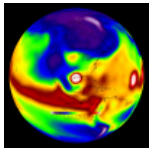
Representation of a plasma from a magnetic fusion energy simulation. Magnetic fields within the plasma are represented as white lines and the temperature is shown as blue/yellow surface (Linda Sugiyama, MIT)



Simulation of the blast resulting from a core collapse supernova. This image, generated by NERSC's Hank Childs, was carried on the TIME Magazine web site following the publication of these simulations.



Various components of a fuel cell from a simulation to help improve the fuel cell membrane (PNNL)



Plot of precipitation on Sept. 9, 1900 from the 20th Century Reanalysis Project, Gilbert Compo (U. Colorado)

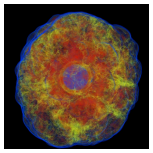


Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

National Energy Research Scientific Computing Center