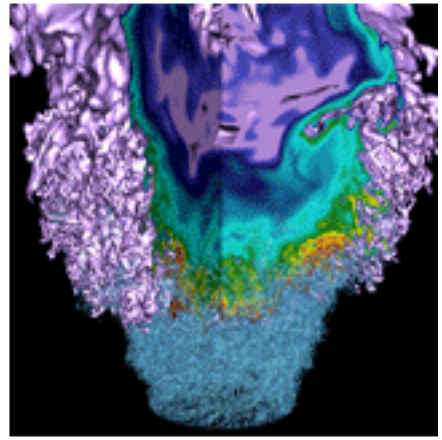
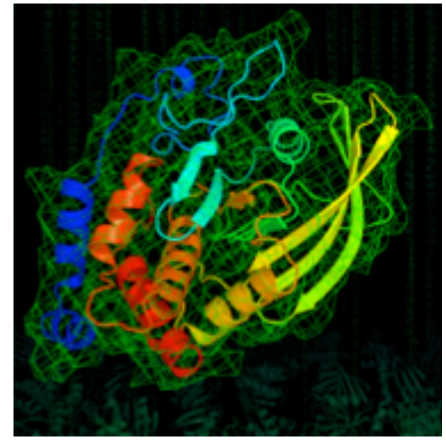
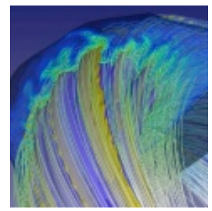
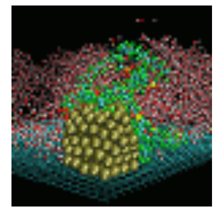
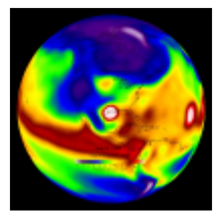
NERSC Science Highlights

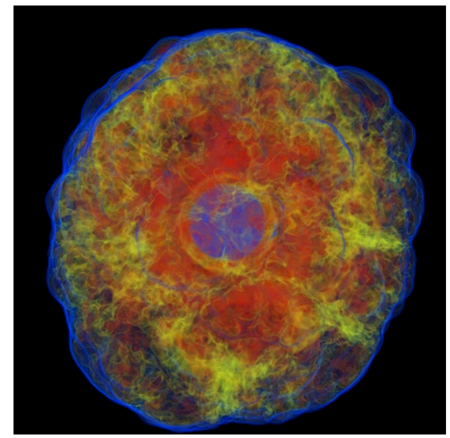












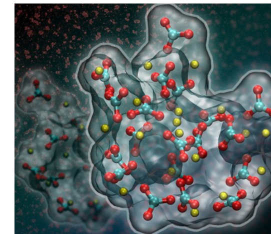
Selected User Accomplishments

September 2013

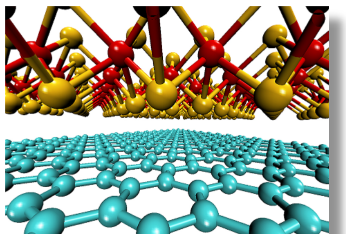
NERSC User Science Highlights

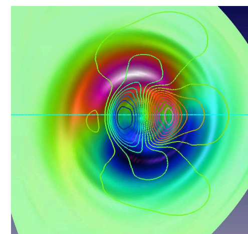
Chemistry
Better catalysts for biofuels via molecular simulation
(D. Mei, PNNL)

Geoscience
New understanding of how crystals form
(A. Wallace, U. Delaware)



Materials
Simulation takes solar power in a new direction: world's thinnest solar cell
(J. Grossman, MIT)





Fusion
Shedding new light on pesky "snakes" that cool magnetic fusion reactions
(L. Sugiyama, MIT)

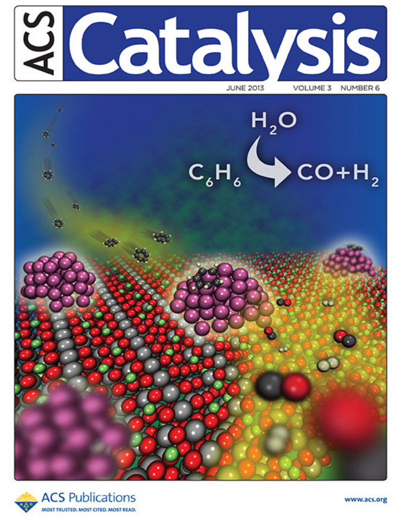
Chemistry
Improving the separation process for Single-Wall Carbon Nanotubes
(A. Striolo, U. Oklahoma)

Life Sciences
Answering fundamental questions about the forces that cause protein misfolding
P. Ghatty (ORNL)

Developing Better Catalysts by Understanding Function at the Molecular Level

NERSC

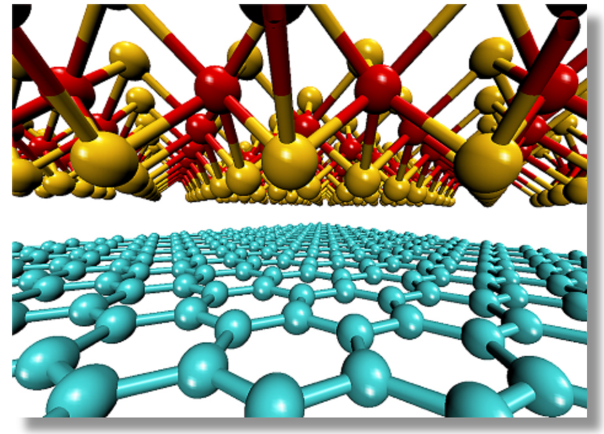
- This work used computation to study catalysts for elimination of impurities produced during biomass gasification – a key part of infrastructure for converting biomass to fuels.
- The computation examined the size of the catalyst and other factors and explained the reaction pathway that takes place in an economically-appealing approach to impurity removal.
- Significance: Provided fundamental understanding of how chemical bonds break and form during a hydrogen-producing reaction and may help improve the speed at which some metal catalysts work.



On the Cover: Artist's conception of a surface on which certain metal nanoparticle catalysts speed up a key chemical process called "reforming," in which organic molecules react with steam to produce hydrogen gas. Computation has helped elucidate the mechanism involved.

Computing the World's Thinnest Solar Cell

- **Accomplishment: First-principles computation has unveiled a new approach for efficient solar energy materials: making them thinner.**
- **Performance for *1-nanometer thick* solar cells – a single atomic layer – is predicted to be at least 1 order of magnitude greater than that of semiconductors in common use today.**
- **Significance: Stacking many of these ultra-thin layers could boost solar efficiency significantly while remaining lightweight.**
- **Suggests that other nanoscale materials hold yet untapped potential for solar energy absorption and conversion.**



Using NERSC supercomputers, MIT researchers demonstrated that an effective solar cell could be made from a stack of two 1-molecule-thick materials: graphene (a one-atom-thick sheet of carbon atoms, shown in blue) and molybdenum disulfide (with molybdenum atoms shown in red and sulfur in yellow). The two sheets together are thousands of times thinner than conventional silicon solar cells.

Study Suggests How to Stabilize Carbon Nanotubes in Water

- **Although carbon nanotubes have attracted enormous research interest, practical application is still hindered by difficulty in separating mixtures of them.**
- **This work used molecular mechanics simulations to study soapy molecules that coat the nanotubes and aid in separation.**
- **Results show how composition of the soapy substance affects ability to preferentially stabilize narrow, rather than wide, carbon nanotubes.**
- **There are many industrial sponsors of this research via the Institute for Applied Surfactant Research; suggests commercial importance of the work.**

On the Cover: Simulation snapshot showing the side-on view of some bulky surfactant molecules (green, white, and red) adsorbed on the surface of two carbon nanotubes. The surfactants help separate the nanotubes in the same way that soaps and detergents separate dirt from clothing and dishes.

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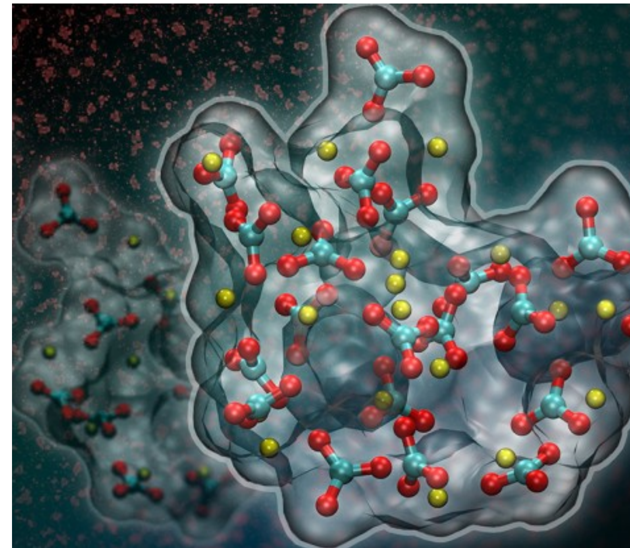
A. Striolo (U. Oklahoma)

Soft Matter, 2013, 9, 3712

BERKELEY LAB

New Theory of Crystallization Falls Out of Computation at NERSC

- **Computation at NERSC is helping to explain one of nature's most important chemical processes: how crystals form.**
- **This work focused on calcium carbonate – a huge player in the planet's carbon cycle.**
- **Molecular dynamics simulations point to formation of large clusters of molecules that form a dense liquid before solidifying into a crystal.**
- **The finding could help us understand how marine organisms respond to changes in seawater chemistry due to rising atmospheric CO_2 levels. Could also aid in predictions of the extent to which geological formations can store carbon underground**



Artistic rendition of a calcium carbonate solution based on NERSC simulation. Results suggest that a dense liquid phase (shown in red in the background and in full atomistic detail in the foreground) forms at the onset of calcium carbonate crystallization.

Science AAAS

Science 23 August 2013: Vol. 341 no. 6148 pp. 885-889

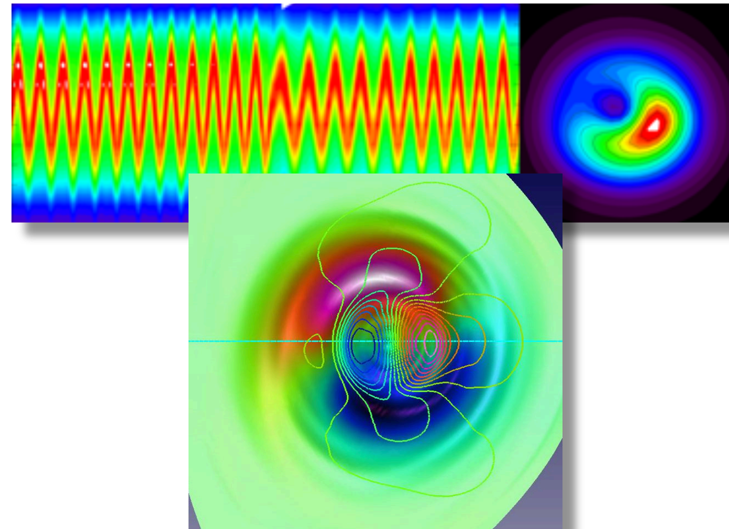
U.S. DEPARTMENT OF ENERGY | Office of Science | BES

PI: A. Wallace (PNNL)

BERKELEY LAB Lawrence Berkeley National Laboratory

New Light Shed on Pesky "Snakes" that Cool Fusion Reactions

- Simulation has helped explain the origin of corkscrew-shaped instabilities called "snakes" that may be important in fusion plasmas such as the International Thermonuclear Experimental Reactor (ITER).
- Although these snakes have been observed in nearly every magnetically confined fusion plasma in the last 25 years, details of their formation and stability have continued to puzzle physicists.
- The NERSC simulations are able to describe the complex, evolving interactions between plasma density and temperature that produce the snake-like patterns. Computation can reproduce details seen in experiments and show that formation of these corkscrew plasma regions cannot be explained as previously thought.

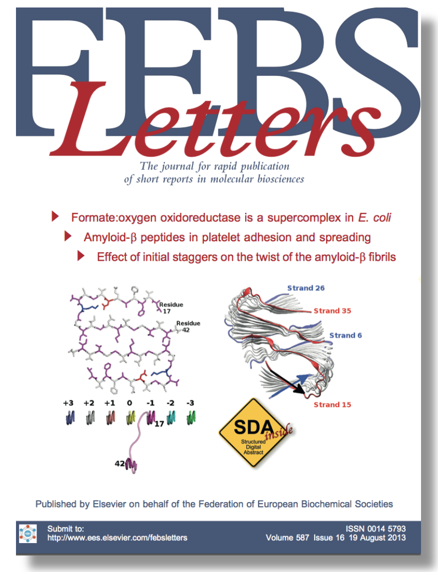


Top: measured time sequence of a snake (side and edge views); Bottom: edge view showing results of a 3-D nonlinear plasma simulation done at NERSC that reproduces the experiment and explains the snake formation.

Physical Review Letters 110, 065006 8 February (2013)

Simulation of Alzheimer's Amyloid Fibril Assembly

- **This work concerns using computation to understand how certain insoluble protein aggregates called "amyloid fibrils" form. These structures are related to a variety of human diseases, especially Alzheimer's.**
- **Fundamental questions about the forces that cause aggregation and key steps involved have long been unanswered.**
- **Results suggest that the twist of the fibrils is strongly affected by relative staggering of different protein chains within the fibril.**
- **The work shows how atomistic simulations can build on experimental efforts to help clarify important details of macromolecular structure.**



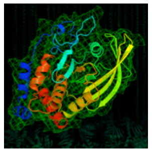
On the Cover: Molecular Dynamics simulations at NERSC have helped explain the physiologically relevant structure of certain misfolded proteins that are associated with the pathology of more than 20 serious human diseases.

Federation of European Biochemical Societies Letters, August 19, 2013
dx.doi.org/10.1016/j.febslet.2013.06.050

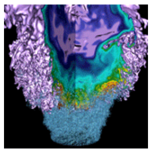
BER

P. Ghatty (ORNL)

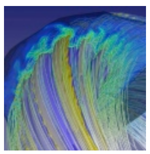
About the Title Slide Images



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)

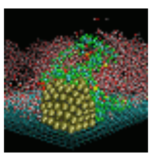


Detailed structure of a flame from a Low swirl burner combustion simulation. Image courtesy of John Bell, LBNL.

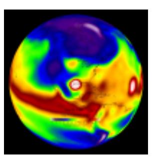


Representation of a plasma from a magnetic fusion energy simulation. Magnetic fields within the plasma are represented as white lines and the temperature is shown as blue/yellow surface (Linda Sugiyama, MIT)

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)

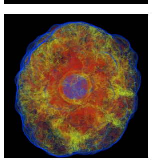


Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

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