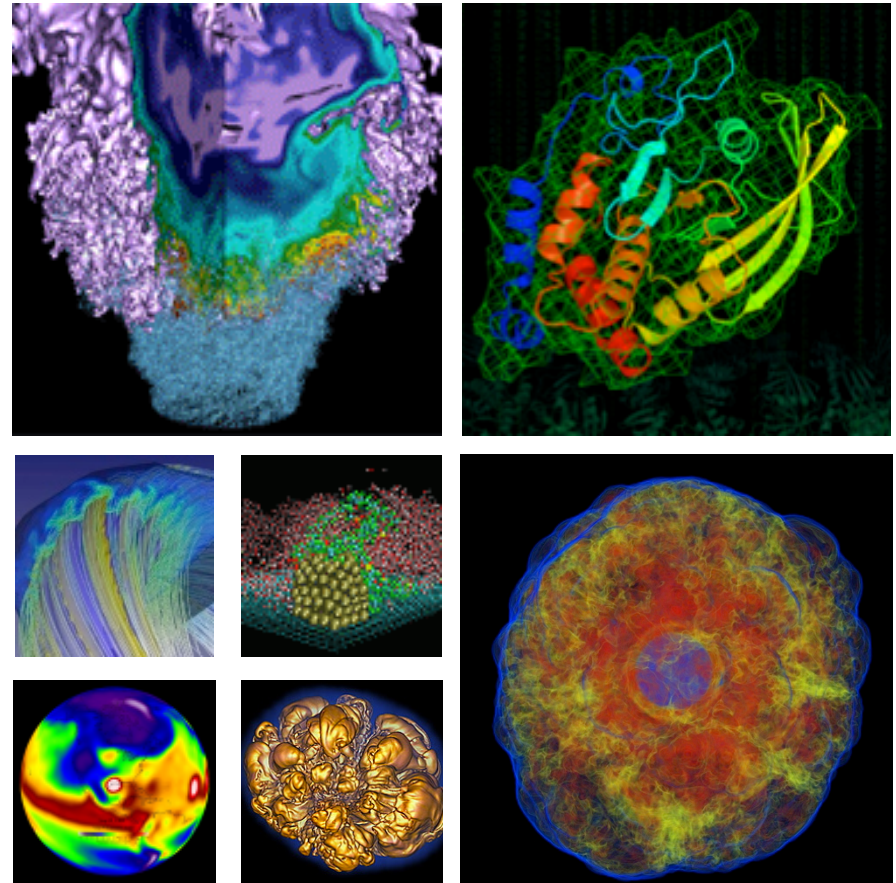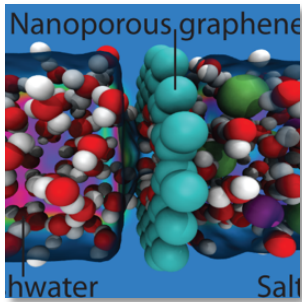# NERSC Science Highlights

Selected User Accomplishments
September / October 2012

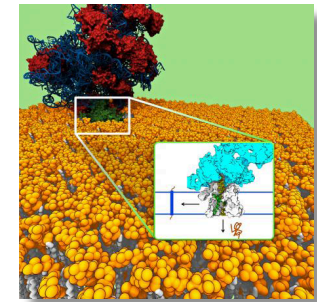# NERSC User Science Highlights

Environment
Using computation to improve water desalination
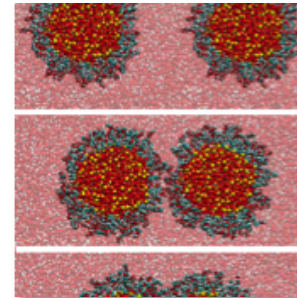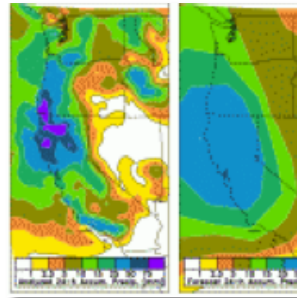**(J. Grossman, MIT)**

Chemistry
Multi-scale simulation sheds light on key protein channel function
(T. Miller, Caltech)

Climate
NOAA reforcast will help improve model accuracy for renewable energy products
(T. Hamill, NOAA)

Materials
Universal viscosity behavior of polymer nanocomposites revealed via 50-day Hopper simulation
(G. Grest, SNL)
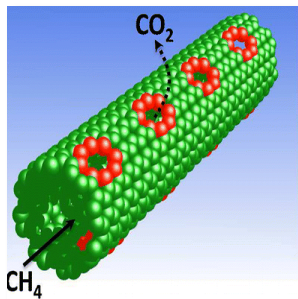
Energy
Simulations show efficient CO_2 removal using hypothetical "windowed" carbon nanotubes
(D. Jiang, ORNL)

High Energy Physics
NERSC users have published the first paper to investigate the implications of the Higgs discovery for Supergravity
(P Nath, Northeastern U.)

September 2012

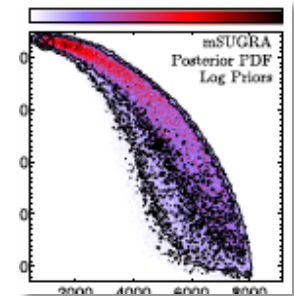# Using Computation to Improve Water Desalination

- **Goal: Systematic computational evaluation of next-generation membranes for clean water technology.**

- **Simulations show why graphene membranes with nano-size pores are able to reject salt ions while letting water flow at permeabilities several orders of magnitude higher than existing membranes.**

- **Suggests that "bottom-up" design of customized nanostructure membrane materials can yield significant improvements over existing technologies for desalination.**
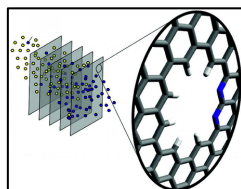
On the Cover: Image from the NERSC simulation was featured on the American Chemical Society's journals home page.

PI: J. Grossman (MIT)

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

BERKELEY LAB
Lawrence Berkeley National Laboratory

Dramatically Increasing Weather Forecast Skill

- **Objective: Reforecast all weather for previous 27 years using NOAA's 2012 state-of-the-art forecast model**

- **Will help improve model accuracy for future forecasts related to renewable energy products (solar, wind, hydro)**

- **Over 700 TB of high-res reforcasted data stored at NERSC. Significant NERSC and ESnet support in transferring ~200 TB back to NOAA, where it is now being enthusiastically used by the community.**

- **NERSC RefCast Scientific Gateway will allow users to access select reforecast days for analytics and reformatting.**

- **ALCC project**
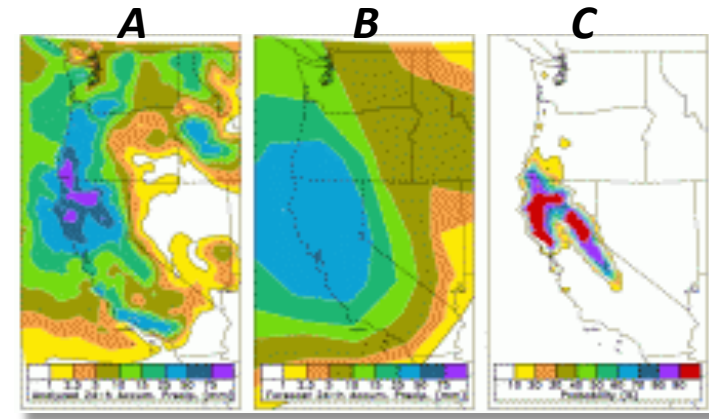
(A) Observed precipitation for 9 January 1995; (B) Original forecast for that day; (C) Reforecast for that day showing dramatically improved model accuracy. The difference is due to systematic error in the original forecast. This example demonstrates why reforecasts are useful in distinguishing between random and model errors and in improving weather/climate guidance.

U.S. DEPARTMENT OF **ENERGY** | Office of Science BER

Pis: T. Hamill, G. Bates (NOAA)

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"Windows of Opportunity" for Efficient CO$_2$ Removal Using Carbon Nanotubes

- **Molecular Dynamics simulations examine the use of a new, hypothetical nanomaterial for carbon dioxide separation.**

  - Natural gas usually contains excess CO$_2$ that must be removed for transmission and heating.

- **The material is a carbon nanotube with molecular size windows or pores on the wall. Simulations suggest a permeance (the degree to which CO$_2$ is removed) that is several orders of magnitude higher than typical polymer membranes.**

  - Also highly selective – 100% methane removal
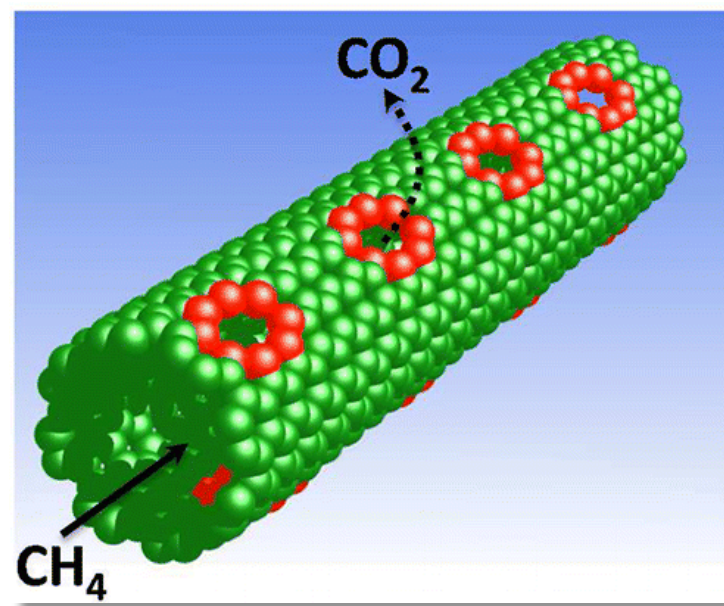
Molecular dynamics simulations at NERSC show how carbon nanotubes fitted with molecular-sized "windows" can efficiently separate CO$_2$ from a CO$_2$/methane mixture.

THE JOURNAL OF PHYSICAL CHEMISTRY Letters   *October 31, 2012*

PI: D. Jiang (ORNL)

BERKELEY LAB
Lawrence Berkeley National Laboratory

Modeling Feat Sheds Light on Protein Channel's Function

- **Chemists at Caltech have managed, for the first time, to simulate the biological function of a *Sec translocon,* a channel that allows specific proteins to pass through membranes.**

    - Simulation spanned nanoseconds-to-minutes timescales, exceeding the scope of earlier simulation efforts by *more than six orders of magnitude*

    - Will help yield a unified picture for this fundamental biological pathway, as well as better understanding of energy transduction in biological systems

    - Additional study carried out at NERSC led to development of a new model to explain anamalous biochemical data for this system (published in PNAS)
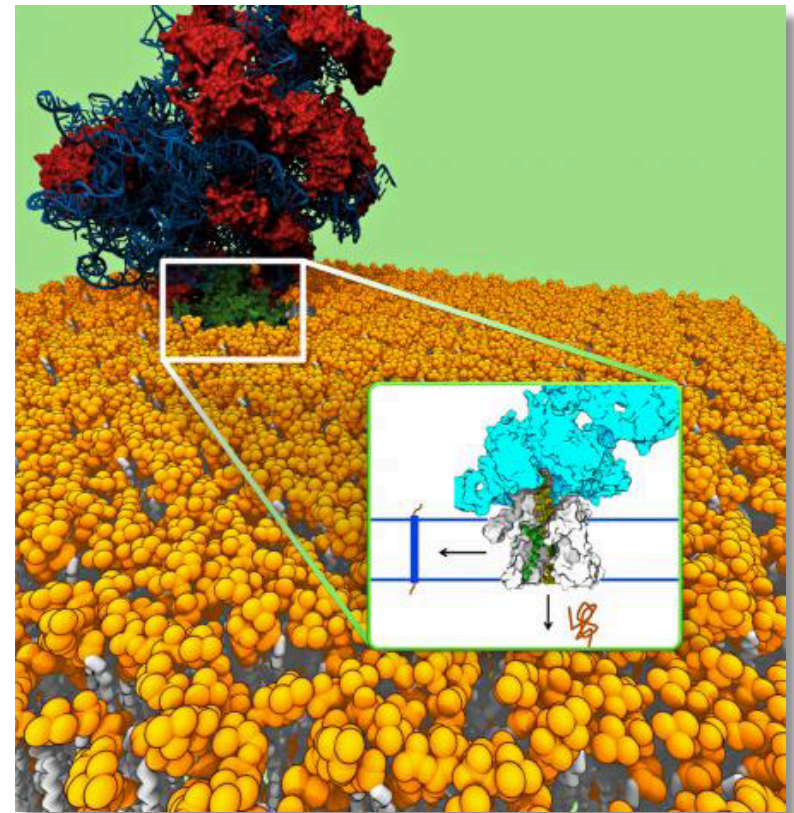
Result from a course-grain molecular dynamics simulation of a ribosome (red-blue) in complex with a translocon channel (green), embedded in a cell membrane (yellow, white).
Cell Reports 2, 927–937, October 25, 2012

B. Zhang, T. Miller (Caltech)

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

BERKELEY LAB
Lawrence Berkeley National Laboratory

Simulations Reveal Universal Viscosity Behavior of Polymer Nanocomposites

- **Objective: Predict the flow behavior of solutions containing coated nanoparticles**

- **Will help to tailor the design & synthesis of a commercially important class of new materials with optical, electrical, magnetic, plasmonic, or sustainable energy applications**

- **50-day simulation on Hopper, 5-6M hours**

- **Nonequilibrium molecular dynamics shows how nanoparticles reduce the viscosity of a polymer melt.**

- **Results provide a quantitative basis for predicting flow behavior (viscosity) as a function of particle & polymer chain size**

- **Editors choice article in PRL**
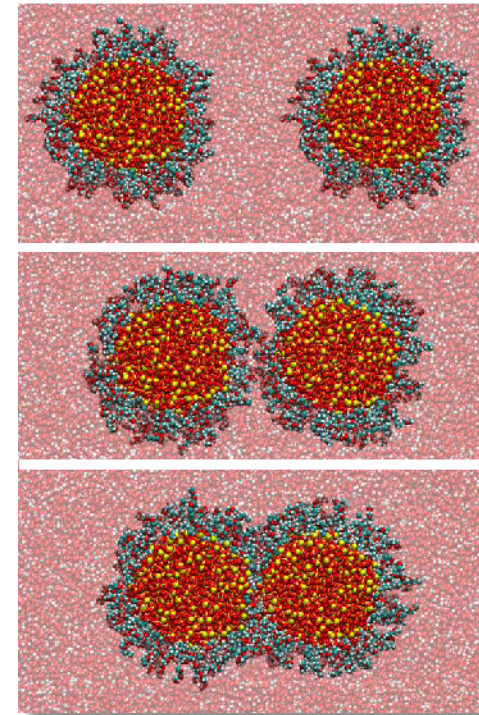
Interaction of two nanoparticles (red/yellow) coated with a polymer (blue). Simulations at NERSC allow a systematic organization of the various forces acting on such a system.

Physical Review Letters
moving physics

PRL 109, 198301 (2012) 9 NOVEMBER 2012

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

BERKELEY LAB
Lawrence Berkeley National Laboratory

Pi: G. Grest (Sandia)

Implications of the Higgs Boson Discovery

- **NERSC users have published the first paper to investigate the implications of the Higgs discovery for Supergravity/ Supersymmetry (SUGRA/SUSY).**

- **The analysis helped identify regions of the mSUGRA parameter space consistent with the Higgs discovery and set lower bounds on sparticle masses.**

  - Also explained why supersymmetric dark matter has not yet been observed: essentially all of the parameter space lies below the sensitivity of current dark matter experiments due to the high Higgs mass.

  - Predicts that the most likely candidates for discovery in the next phase of LHC runs are the gluino, chargino and the stop.

Calculated probability density distribution (left column) and likelihood profile (right) in the planes of the phenomenologically important sparticle masses. From top to bottom: the gluino–squark mass plane; the squark–chargino mass plane; and the stau–stop mass plane

PHYSICS LETTERS B
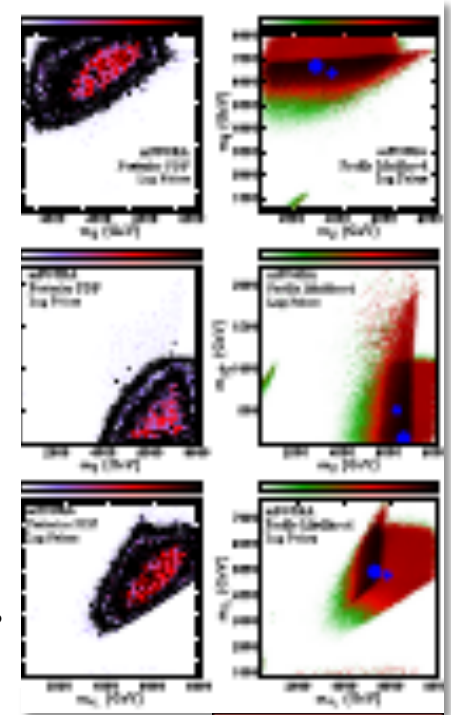
in press; doi 10.1016/j.physletb.2012.09.007

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

PI: P. Nath (Northeastern U.)

BERKELEY LAB
Lawrence Berkeley National Laboratory
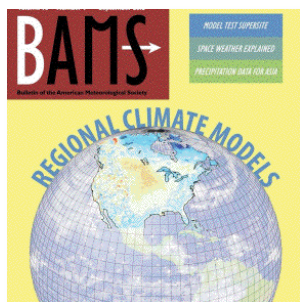
NERSC User Science Highlights

Climate

NERSC resources used to help extend, validate, and optimize new regional climate–weather research and forecasting model
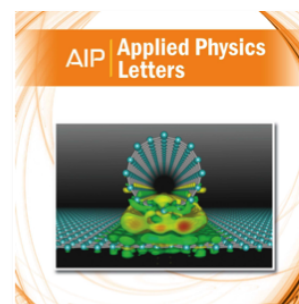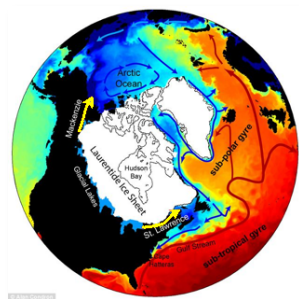**(X.-Z. Liang, U. Maryland)**

Chemistry

Simulations reveal key fuel cell membrane characteristics
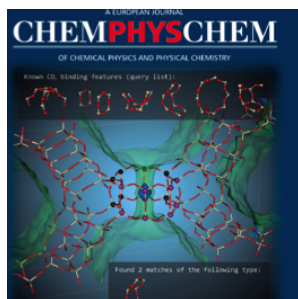**(T. Miller, Caltech)**

Climate

Modeling reveals how oceans plunged the planet into a catastrophic big freeze
(A. Condron, U. Mass)

Materials

Calculations suggest promise for transistors made of graphene and carbon nanotubes
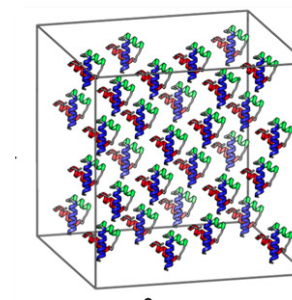**(K. Varga, Vanderbilt U.)**

Energy

New approach screens a database of potential gas separation materials 65 times faster than brute force methods
**(B. Smit, Berkeley)**

Proteins

"Test-tube" simulations explore 32 copies of a protein unfolding simultaneously
(V. Daggett, U. Washington)

October 2012

A Climate Extension to the Weather Research and Forecasting Model (CWRF)

- **Development of a cost-effective Cloud-Aerosol-Radiation (CAR) ensemble representation**
  - vital for accurate climate modeling at regional to local scales

- **NERSC resources were used to –**
  - check the physics expression of the model
  - check the performance
  - improve the model

- **New CAR interactions are fully coupled with the state-of-the-art mesoscale non-hydrostatic Climate-Weather Research and Forecasting model (CWRF)**
  - About 2,000 CWRF-model-year experiments carried out
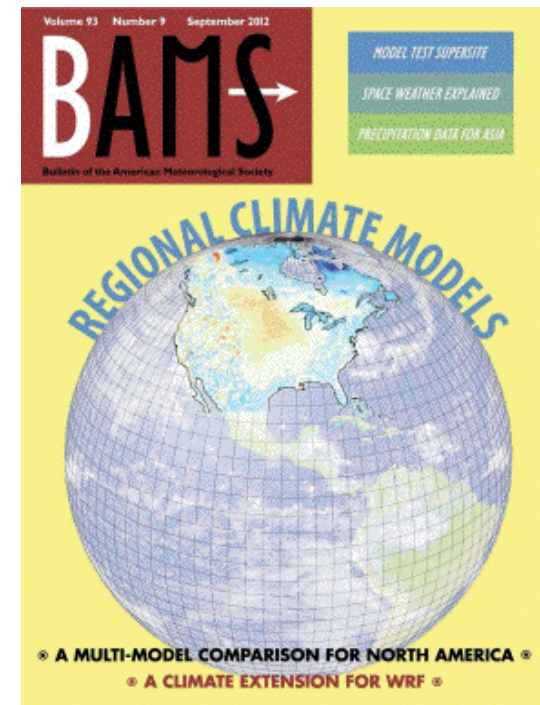
On the Cover: September issue of the Bulletin of the American Meteorological Society featuring CWRF

*Bull. Amer. Meteor. Soc., 93, 1363–1387 (2012)*

Pi: Xin-Zhong Liang (U. Maryland)

Modeling Reveals How Oceans Plunged the Planet into a Catastrophic Big Freeze

NeRSC

- **Discovery that Earth's last major cold spell 13,000 years ago was likely caused by catastrophic deluge of meltwater from northwest Canada into the Arctic ocean**

- **Findings point to the Arctic as a primary trigger for climate change.**
  - Suppression of Atlantic Meridional Overturning Circulation from melting ice could suddenly alter the modern climate

- **NERSC resources were used to develop a sophisticated iceberg model, incorporate it into the MITgcm coupled model, and for 20-50-year high-resolution integrations.**
  - Allowed 20X greater resolution than previous study; ability to capture smaller scale, faster moving coastal currents played a key role
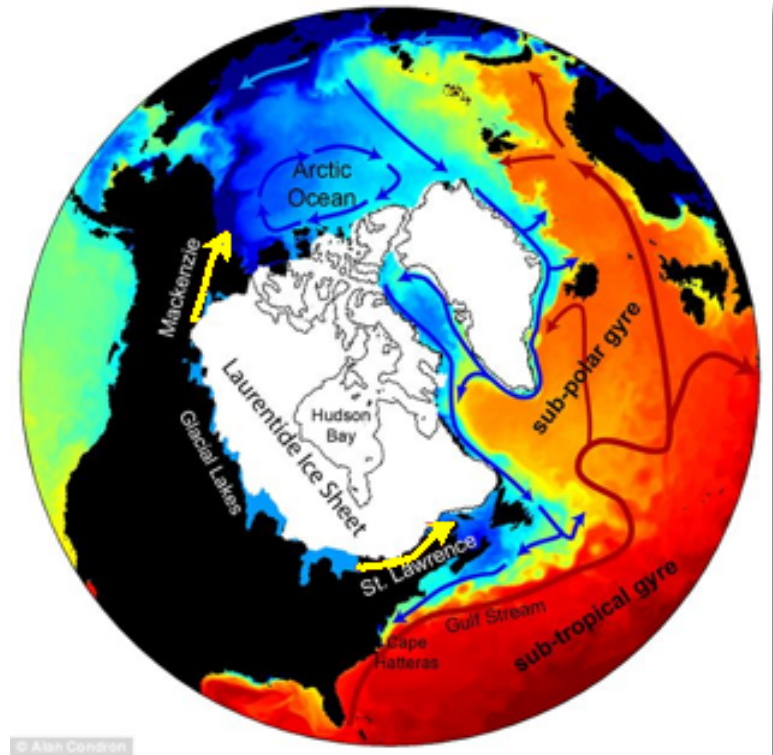
This graph of ocean salinity shows drainage pathways (yellow arrows) for meltwater stored in glacial lakes at the southern margin of the Laurentide Ice Sheet. Simulations at NERSC suggest that meltwater discharge via the Mackenzie Valley into the Arctic Ocean, rather than from the St. Lawrence Valley, was more likely to have triggered the famous Younger Dryas cooling.

PNAS Online Nov. 5, 2012

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

BERKELEY LAB
Lawrence Berkeley National Laboratory

Pi: A. Condron (U. Mass.)

Efficient Discovery of Porous Materials for Gas Separation and Storage

- **Promising materials for removal of CO_2 and other molecules are being discovered using a new computationally-efficient method**
  - Uses *ab-initio* geometry-based screening of material void spaces in existing zeolite databases.

- **Allows materials discovery using databases an order of magnitude larger than before**

- **Avoids expensive computer simulations and unneccesary lab synthesis of candidates that turn out to be suboptimal**

On the Cover: A potential binding site (blue, center) is shown to be correctly identified for adsorption of CO_2

Martin, R.L.; Willems, T.F.; Lin, L.-C.; Kim, J.; Swisher, J.A.; Smit, B.; Haranczyk, M. ChemPhysChem 2012, 13 (16), 3595-3597.

Center for Gas Separations Relevant to Clean Energy Technologies

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

BERKELEY LAB
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PI: B. Smit (Berkeley)

Simulations Reveal Key Fuel Cell Membrane Characteristics

- **Molecular Dynamics simulations explain key differences between Nafion®, the current membrane of choice for fuel cells, and a key, new membrane candidate.**

- **Modeling sheds light on pore structure, water percolation, and ion and molecule transport in membranes**

- **Able to follow the precise pathway a proton takes through the membrane**

- **Fuel cells are promising – but costly – energy conversion devices.**

  - The challenge is to develop a relatively inexpensive and robust membrane that conducts protons effectively.   This work is viewed as a first step.

  - Used NERSC + EMSL
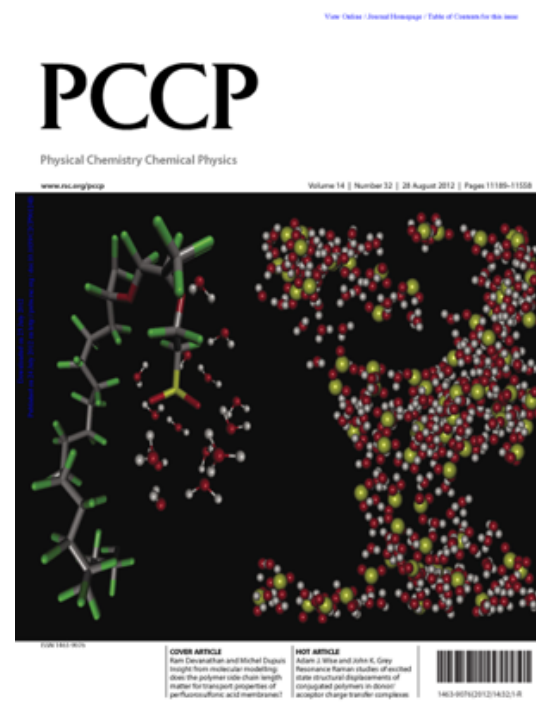
On the Cover: snapshot from a NERSC simulation examining transport properties of fuel cell membranes

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

BERKELEY LAB — Lawrence Berkeley National Laboratory

PI: R. Devanathan (PNNL)

Calculations Suggest Promise for Graphene-Nanotube Transistors

- **First-principles electronic structure and transport study of the junction between a carbon nanotube and graphene.**
  - The quality of the contact between the materials is a key issue for ultra-fast, low power nano-electronic integrated circuits.
- **Calculations provide qualitative insight into the role the junction plays in determining current-voltage response.**
  - Results explain conflicting experimental data, suggest the suitability of the junctions for device applications, and propose paths for future experiments.
  - NERSC resources were essential due to the large k-point sampling and simulation cell size in these calculations.
  - Key NERSC consulting support for SIESTA and GPAW codes
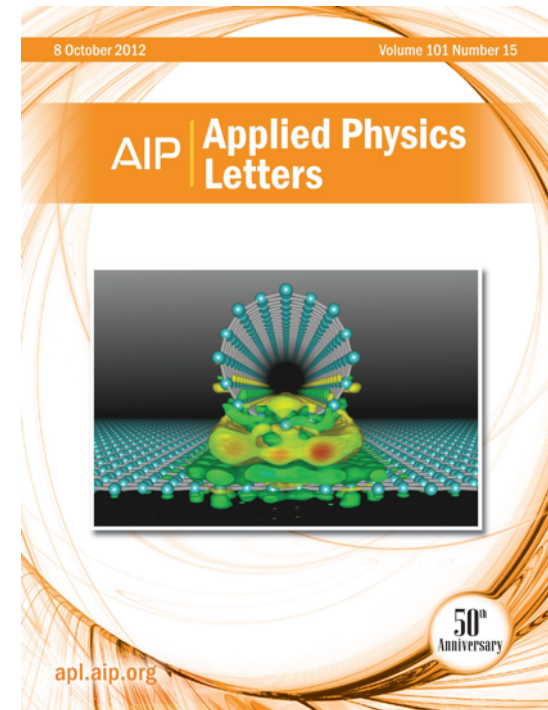
On the Cover: Image showing electronic charge density between a graphene sheet and a nanotube computed at NERSC.

Applied Physics Letters 101, 153501 (2012)

K. Varga, Brandon Cook (Vanderbilt U.)

Computer as Laboratory: Test-Tube Simulations of Protein Unfolding

- **Molecular dynamics simulation of protein unfolding using 32 copies of the protein simultaneously**
  - to explore effects of neighboring molecules on the unfolding/folding pathway: "test-tube" simulations
  - These effects are largely ignored experimentally and have never been modeled computationally.
  - Showed that intermolecular interactions have little effect on the folding/unfolding pathway.
  - Results support using the common single-molecule approach; also provide insight into interactions that occur as proteins aggregate at high temperature
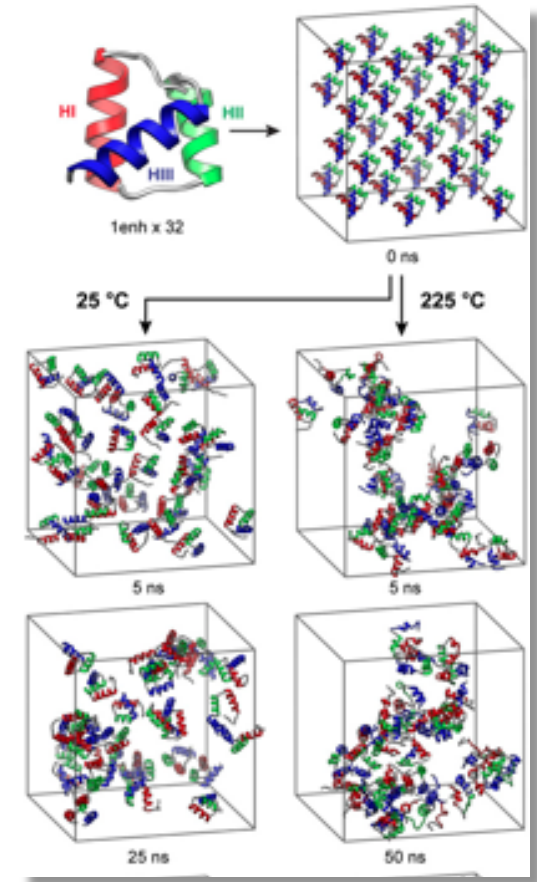
A single molecule of the protein studied, 32 replications of it, and folding pathways for the 32 copies at two different temperatures.
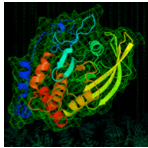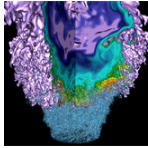
PNAS October 30, 2012

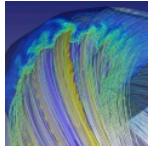**PI: V. Daggett (U. Washington)**

# 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)
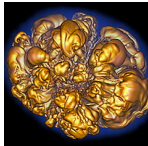
Simulation of the blast resulting from a core collapse supernova. This image, generated by NERSC's Hank Childs, was carried on the TIME Magazine web site following the publication of these simulations.
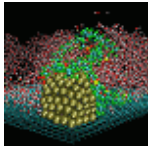
Various components of a fuel cell from a simulation to help improve the fuel cell membrane (PNNL)
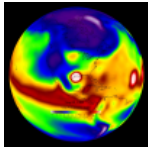
Plot of precipitation on Sept. 9, 1900 from the 20th Century Reanalysis Project, Gilbert Compo (U. Colorado)
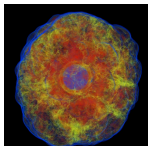
Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

National Energy Research Scientific Computing Center