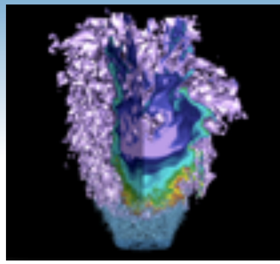
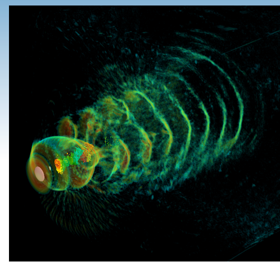
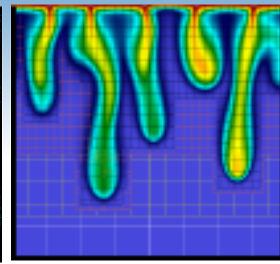
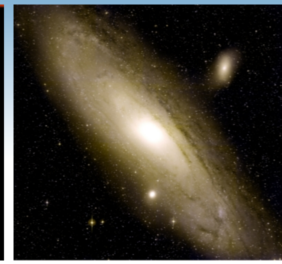
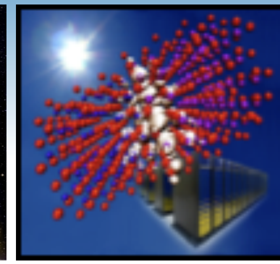
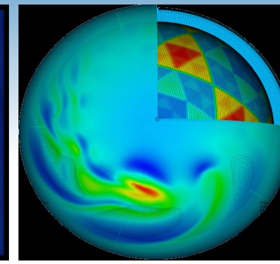







NERSC Science Highlights

A selection of science results produced by NERSC users

December, 2010

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC National Energy Research Scientific Computing Center

BERKELEY LAB

NERSC User Scientific Accomplishments December, 2010

Materials

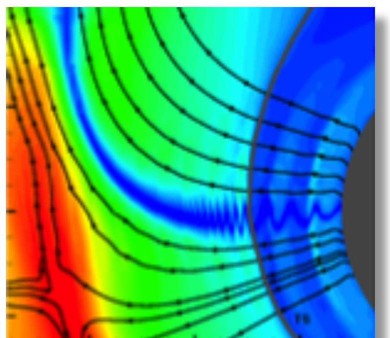
Simulations done at NERSC helped validate key new experimental technique that allows researchers to "see" individual atoms
(Pennycook, ORNL)

Energy Resources

First-principles simulations performed on Franklin revealed the mechanism of a full catalytic cycle for low-temperature activation of methane on small gold clusters.
(U. Landman, Georgia Tech)

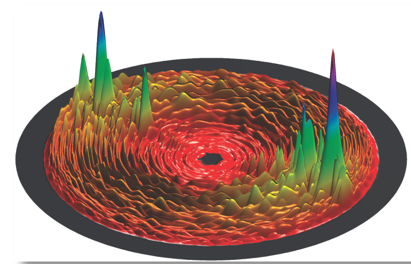
Fusion

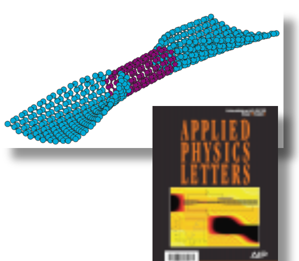
Study by award-winning researcher explained magnetic reconnection phenomenon observed by *Voyager* spacecrafts.
(J. Drake, U. Maryland)



Chemistry

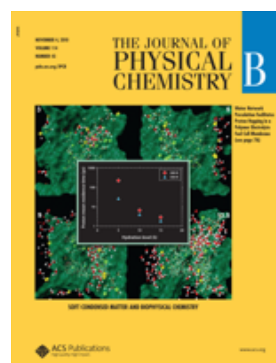
Quantum dynamics of a reaction important to both combustion and ozone depletion were revealed using a newly parallel method developed at NERSC.
(H. Guo, Univ. of New Mexico)





Low-Power Computing

Quantum transport simulations may lead to discovery of nano-devices that can act as transistors.
(S. Salahuddin, UC Berkeley)



Fuel Cells

Simulations may lead the way toward rational design of polymer membranes, key components of fuel cells.
(M. Dupuis, PNNL)

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Simulation Helps Validate Key New Experimental Technique

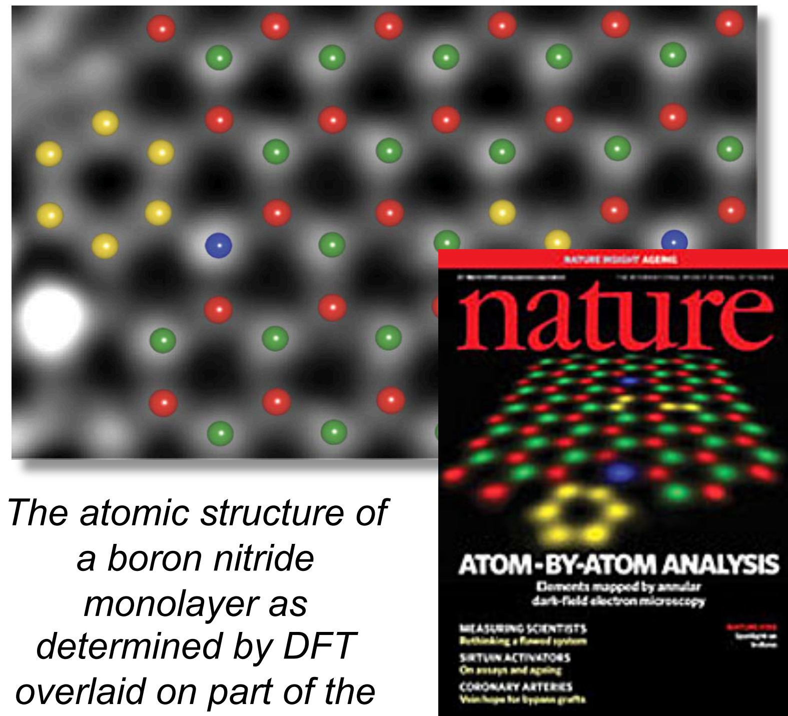
Objective: **Investigate atomic-scale structure of complex materials in conjunction with microscopy experiments.**

Implications: **Combination of simulation and experiment represents a powerful means of uncovering material structure.**

Accomplishments: **New technique is the first where scientists can actually "see" individual atoms of boron, carbon and nitrogen.**

- **Density Functional Theory (DFT) simulations (on Franklin) validated the results.**
  - **Helped bound the limit of the new technique.**
- **The new high-resolution images will allow researchers to design more accurate simulations.**

Pantalides, Pennycook, et al., (ORNL)



The atomic structure of a boron nitride monolayer as determined by DFT overlaid on part of the experimental image. Red, B; yellow, C; green, N; blue, O.

Nature, 25 March 2010 (cover story)

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Quantum Dynamics Revealed

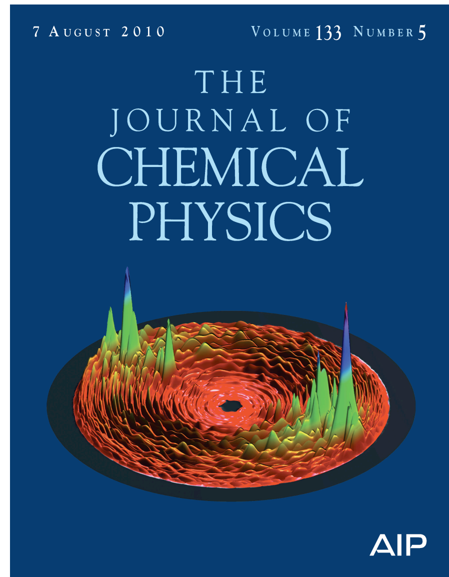
Objective: **Study detailed quantum dynamics of elementary chemical reactions in the gas phase and on surfaces.**

Implications: **These elementary reactions are often at the heart of important processes in combustion and catalysis.**

- ***Accomplishments:*** **Detailed calculations of O+OH➔H+O_2, which is the reverse of the most important combustion reaction and is also important for ozone destruction, shed light on long-standing questions about the statistical nature of the reaction dynamics.**
- **Results will serve as a benchmark for more approximate treatments.**

NERSC: **Codes using OpenMP parallelism for calculating both total and differential cross sections were developed on Franklin and Hopper; NERSC NISE award, 2010**

H. Guo (UNM)



The cover image shows a polar-coordinates plot of differential cross sections for the O+OH reaction at 150meV of collision energy. The article was one of the top-20 most downloaded papers from this issue.

State-to-state quantum dynamics of the $O(^3P)+OH(^2\Pi)\rightarrow H(^2S)+O_2(^3\Sigma_g^-)$ reaction

Journal of Chemical Physics 133, 054302, August 7, 2010 (cover story)

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Nanocatalysis: "Small *is* Different"

Objective: Use quantum and classical simulation to investigate catalysis of methane reactions.

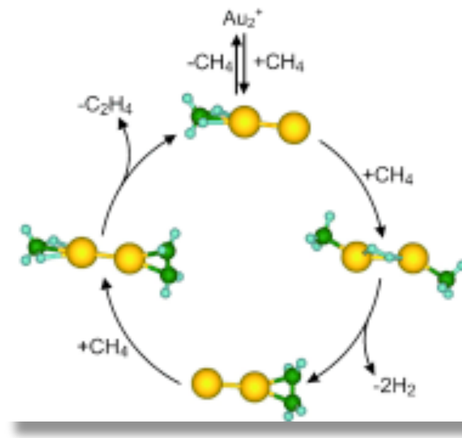
Implications: Aid in conversion of methane into valuable chemical products and fuels.

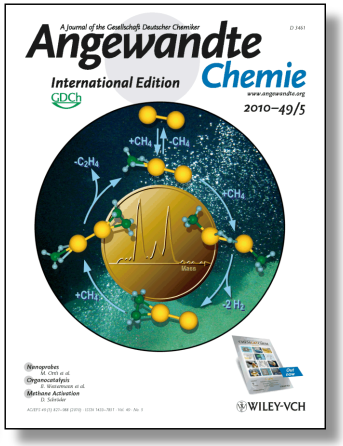
Accomplishments: First-principles theoretical calculations played a leading role in discovering a full catalytic cycle for low-temperature activation of methane on free gold atoms.

- Showed that small metal clusters adsorbed on support materials exhibit unique catalytic properties.
- Demonstrated how to gain deep insights into complex chemical processes through coordinated state-of-the-art experimental and theoretical techniques.

NERSC: Accomplished with .ca 45,000 hours on Franklin using ~800 cores per job in 2009.

U. Landman, R. Barnett (GaTech)





Individual steps in a full catalytic cycle for methane (CH_4) conversion to ethylene (C_2H_4) on gold atoms discovered using first-principles theoretical studies on Franklin at NERSC

Angewandte Chemie International Edition Vol 49 (5) 980–983, January 25, 2010 (cover story)

Ultra Low-Power Computing?

Objective: **Simulate factors that affect nanoscale quantum transport.**

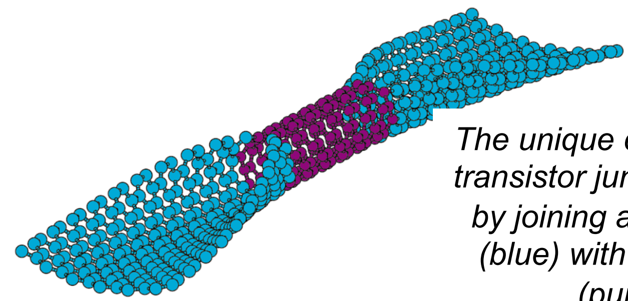
Implications: **May lead to discovery of nano-devices that can act as transistors, maintaining fast switching speeds but drastically reducing voltage requirements.**

Accomplishments: **Simulations showed that the interface between a graphene nanoribbon and a carbon nanotube results in a unique transistor structure.**

- **The device acts like a tunneling transistor at low voltages but allows a large "on" current at high voltages.**

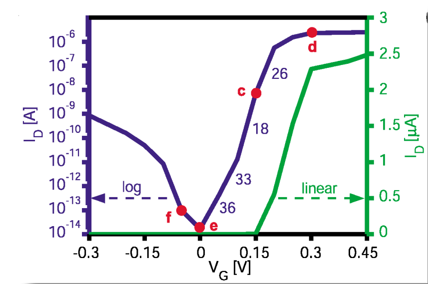
- ***NERSC***: **Work done mostly on Jacquard using a small allocation (15k hours) in 2009. NISE award in 2010 is enabling a custom electronic transport code to scale to 8,000+ cores along with application to new areas.**

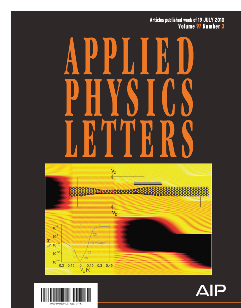
Y. Yoon, S. Salahuddin (UCB)



The unique carbon-based transistor junction created by joining a nanoribbon (blue) with a nanotube (purple).

Simulation results showing that electric current (purple line) increases by 4 orders of magnitude with a change in voltage of only 100 mV.





Appl. Phys. Lett. 97, July 19,2010, 033102 (cover story)

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NERSC Designing Fuel Cell Membranes

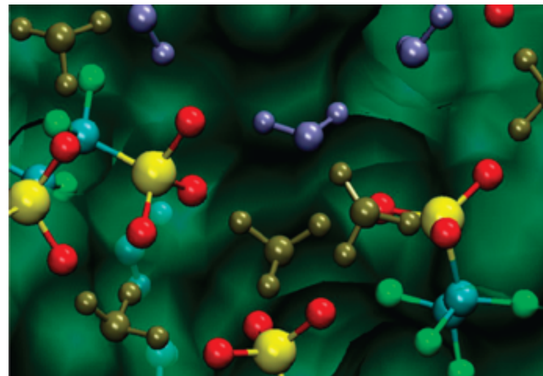
Objective: **Fundamental understanding of proton transport to enable rational design of fuel cell membranes.**

Implications: **Membranes are key fuel cell components: they conduct charge while separating the fuel cell reactants. But no existing membrane exhibits all properties necessary for widespread use.**

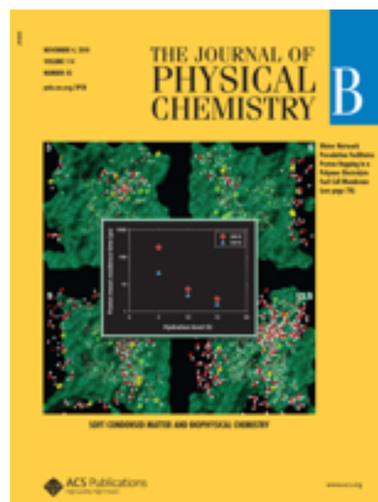
Accomplishments: **Performed classical and quantum simulations of the common membrane "Nafion" as a function of hydration level.**

- **Showed how water percolation affects proton hopping across the membrane and quantified hydration level to achieve it.**
- **Results could lead to design of future polymer membrane materials that have lower uptake of water and yet offer faster proton transfer and transport.**

R. Davanathan, M. Dupuis, et al. (PNNL)



A portion of the membrane simulated, showing water, hydronium ion, and different parts of the Nafion polymer.



J. Phys. Chem. B, 114, 13681–13690, November 4, 2010 (cover story)

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Magnetic Reconnection and Anomalous Cosmic Rays

Objective: Complete understanding of reconnection: how magnetic fields change topology and convert magnetic energy to kinetic and thermal energy.

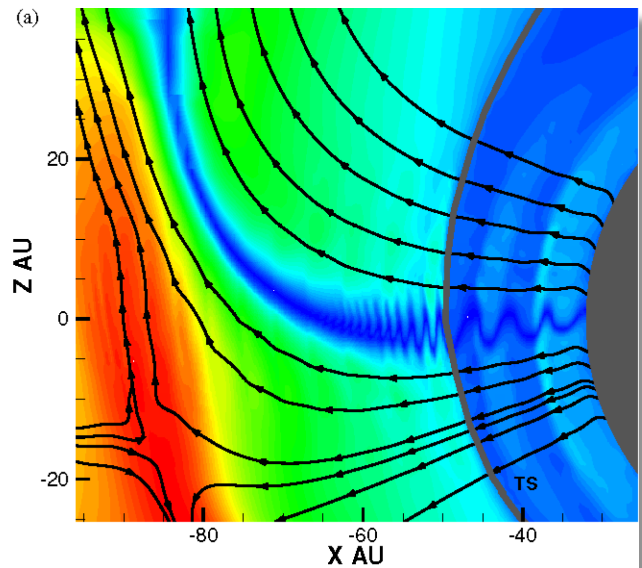
Implications: Has broad importance in space (e.g. solar flares), astrophysics, and fusion experiment plasmas.

Accomplishments: Provided explanation for surprising *Voyager 1* & *2* spacecraft observation of Anomalous Cosmic Rays (ACRs: ions with energies just below galactic cosmic rays).

- Required both magnetohydrodynamic (MHD) and particle-in-cell (PIC) methods.
- Drake is 2010 winner of APS Maxwell Award for Plasma Physics.

- ***NERSC***: Simulations use 1,024-8,192 cores (Franklin).

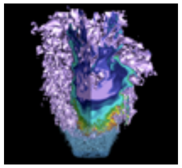
J. F. Drake, et al. (U. Maryland)



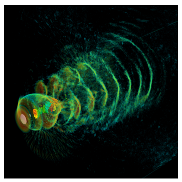
2-D view of the magnetic field and flow streamlines from a high-resolution, 3-dimensional MHD simulation of the interaction of the solar wind with the interstellar medium, interplanetary and interstellar magnetic field, and ionized and neutral H atoms.

The Astrophysical Journal (APS) 709:963–974, February 1, 2010

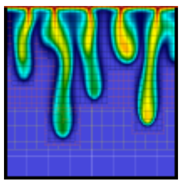
About the Cover Images



Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. Simulated using an adaptive projection code. Image courtesy of John Bell, LBNL.

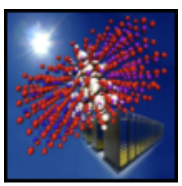


Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour LOASIS experiment simulation using VORPAL by Cameron Geddes, LBNL. Image courtesy of Cameron Geddes..

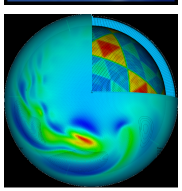


Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving the security of CO_2 storage. Image courtesy of George Pau, LBNL

False-color image of the Andromeda Galaxy created by layering 400 individual images captured by the Palomar Transient Factory (PFT) camera in February 2009. NERSC systems analyzing the PTF data are capable of discovering cosmic transients in real time. Image courtesy of Peter Nugent, LBNL.



The exciton wave function (the white isosurface) at the interface of a ZnS/ZnO nanorod. Simulations performed on a Cray XT4 at NERSC, also shown. Image courtesy of Lin-Wang Wang, LBNL.



Simulation of a global cloud resolving model (GCRM). This image is a composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid. Image courtesy of Professor David Randall, Colorado State University.