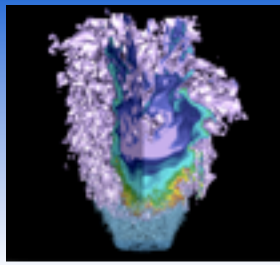
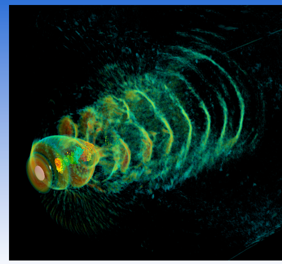
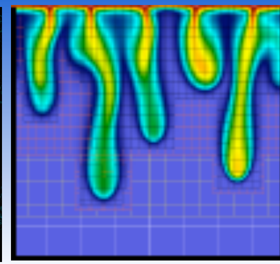
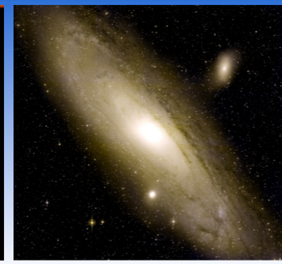
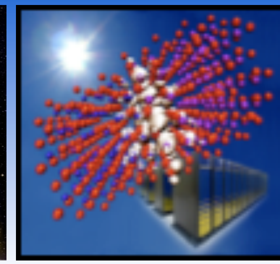
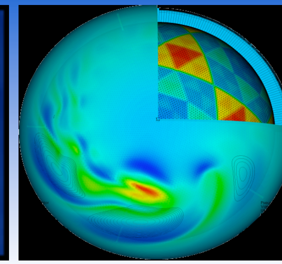
     

NERSC Science Highlights

A selection of scientific results produced by NERSC users.

June, 2010

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC

BERKELEY LAB

Silicon Uncommon in Deep Earth

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Investigate structural properties of silica (SiO_2) and other materials under extreme conditions.

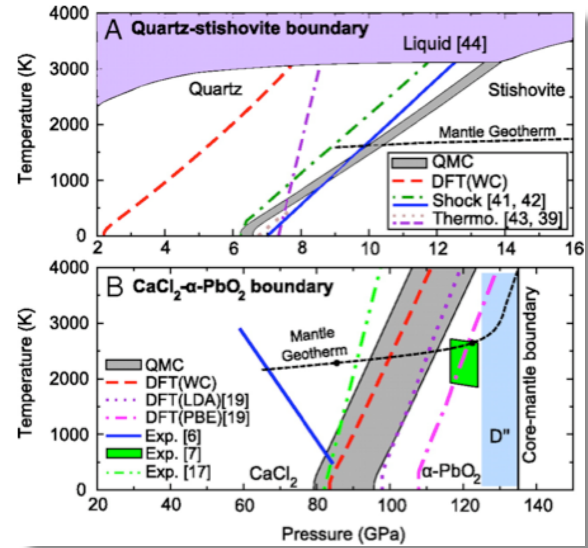
Implications: One of the most ubiquitous and important minerals, SiO_2 is used in ceramics, electronics, and glass. But its abundance and role in the structure and dynamics of deep Earth is still unknown.

Accomplishments: Quantum Monte Carlo results suggest that Silica populates Earth only superficially; it's relatively uncommon deep within the Earth.

- Results document improved accuracy and reliability of QMC relative to the more common and efficient Density Functional Theory method; increased role seen.

NERSC: Key pre-production FranklinQC user, 3Mhours; CASINO code; 4-4k cores, avg. 420

J. Wilkins, K. Driver (OSU)



Computed phase diagrams that reveal at which temperature (vertical) and pressure (horizontal) within the Earth the various forms of silica are stable. Results suggest that there is little or no free silica in the bulk of the lower mantle.

Proceedings of the National Academy of Sciences, May 10 online early edition

First-Ever Antimatter Hypernucleus

Objective: Simulation and data analysis supporting the Brookhaven STAR high-energy heavy nuclei collision experiments.

Implications: Recreate what is believed to be the conditions in the universe just microseconds after the Big Bang.

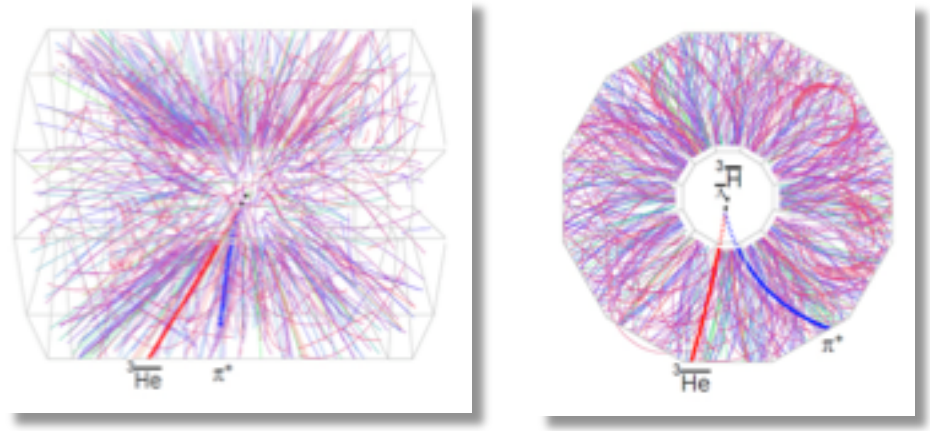
Accomplishments: Detection of antimatter nuclei containing strange quarks for the first time – an antihypertriton, consisting of an antiproton, an antineutron and an antilambda particle

- Involved analyzing over 100M collisions and their products.

NERSC: PDSF is the main facility for embedding production, a process critical to the analysis of STAR data.

- Over 1PB of data are expected to be stored on NERSC HPSS.

N. Xu (LBNL) *et al.*



A typical event in the STAR detector that includes the production and decay of an antihypertriton candidate The dashed black line is the trajectory of the candidate, which cannot be directly measured. The heavy red and blue lines are the trajectories of an antihelium nucleus and a pion, decay daughters which are directly measured.

Science 2 April 2010
Vol. 328. no. 5974, pp. 58 - 62

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

BERKELEY LAB

Why Neon is Missing from Jupiter's Atmosphere

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **First-principles study of high pressure, dense water, oxygen, & hydrogen**

Implications: **Understanding materials under extreme conditions that cannot be reached with lab experiments.**

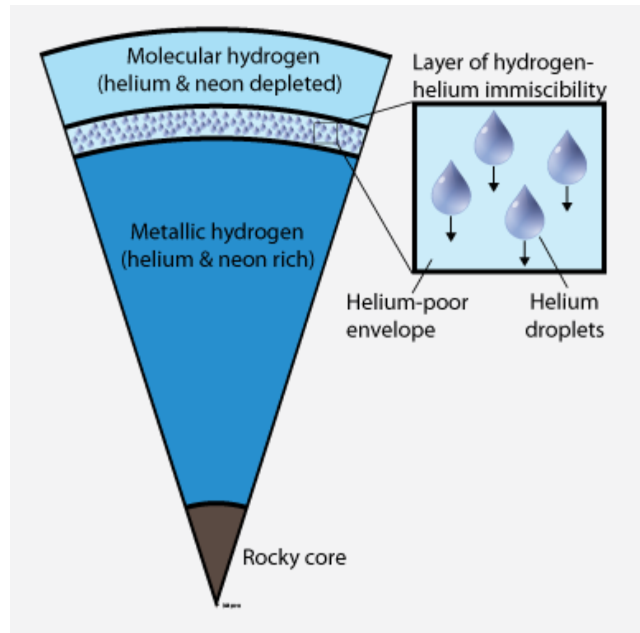
Accomplishments: **Depletion in neon in Jupiter's atmosphere, observed by the Galileo probe, is explained by sequestration of neon into helium-rich droplets within the postulated hydrogen-helium immiscibility layer of the planet's interior.**

- **Provides strong, though indirect, evidence of linkage to helium rain.**

NERSC: **"We are very grateful to NERSC for providing us with CPU hours in the beginning stages of our research. This time allowed us to run a large number of relatively short runs at a critical stage of our research."**

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

H. Wilson, B. Militzer (UC B)



Jupiter's interior. Simulations show that helium rain occurs in the immiscibility layer and depletes the upper layer of both helium and neon

Physical Review Letters
March 26, 2010

BERKELEY LAB

Mysteries of Massive, Young, Star-Forming Galaxies Explained

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Explain galaxy formation and evolution via high-resolution gas hydrodynamic simulations.

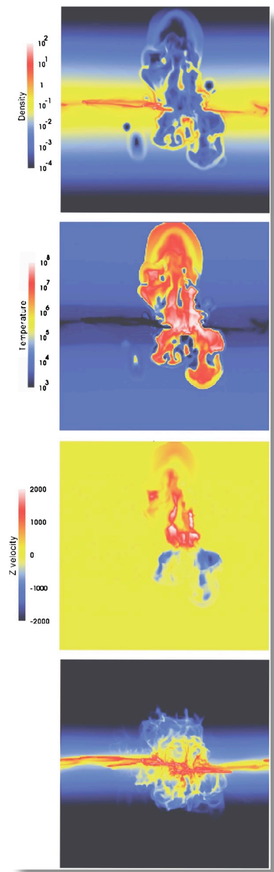
D. Ceverino, A. Klypin (NMSU)

Implications: Help solve some remaining mysteries of the standard model of big bang cosmology.

Accomplishments: Results help explain the formation of huge star-forming galaxies that date from the early universe.

- Best physics, highest resolution simulations of galaxy formation to date.
- Identified role of small-scale supernovae explosions and stellar wind feedback
    - Showed where and how energy from massive stars is released

- ***NERSC***: Used mostly single-node Bassi, some Franklin (248 cores)



Simulations showing the formation of a galactic "chimney" that happens when the energy input of stellar superclusters causes gases to shoot upwards at speeds up to 1000 km per second at temperatures reaching 100 million Kelvin. These edge-on slices through the simulation show density, temperature, and velocity. Small bubbles of hot gas in the field (visible in the top two frames) are the result of stellar feedback from runaway stars. The elucidation of the feedback mechanism, a result of the resolution and physics models employed, is one of the key results of this work.

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The Astrophysical Journal 695 (2009) 292

BERKELEY LAB

First-Principles Modeling Reveals Details of Distant Metal-Water Bonds

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Objective: Use molecular modeling to understand hydration structure of metal ions related to biogeochemical activity in subsurface environments.

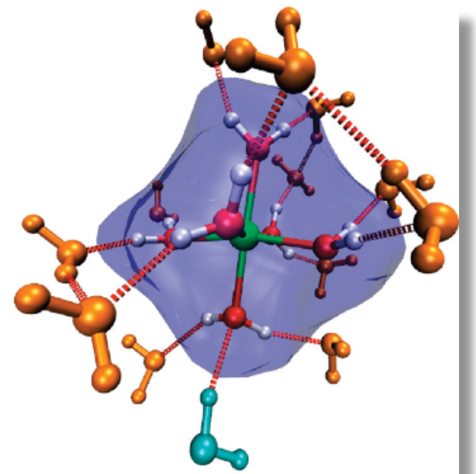
Implications: Dissolved metals play a role in mineral extraction, toxic material transport and biochemical activation but their structure is difficult to obtain experimentally.

Accomplishments: System with one iron ion and 64 H_2O molecules (517 electrons) simulated for 30 picoseconds

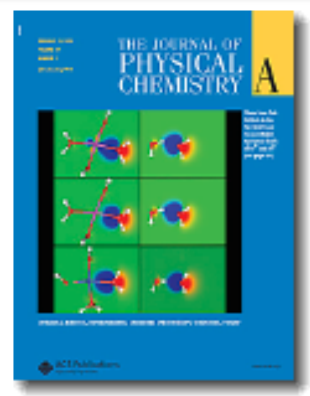
- 5X longer, 2X more H_2O's than previously
- Demonstrated importance of first-principles approach in these studies.

NERSC: Computations done using NWChem on Franklin (~ 272 cores) / Bassi (~ 112 cores) and elsewhere; collaboration with NERSC on NWChem port, debugging for Cray XT

S. Bogatko, E. Bylaska, (PNNL)
J. Weare (UCSD)



Hydrogen bonds from the simulation. The key result from this work is the elucidation of the structure and bonding of outer "shell" water molecules (those outside the purple area).



The work was chosen for the cover story in the January 15, 2010 issue of the Journal of Physical Chemistry (A)

Thermophillic Protein Stability Explained

Objective: Complete understanding of protein dynamics via simulation.

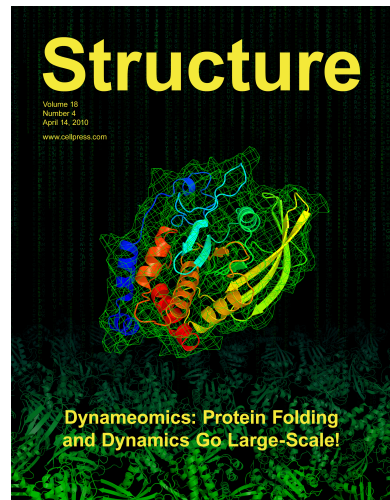
Implications: A broad knowledgebase of structural pathways to support research in bioenergy production, environmental remediation, and carbon cycling.

Accomplishments: Helped explain the stability of thermophilic proteins (proteins from organisms that thrive at high temperatures, up to ~176 °F).

- Simulation results for >2,000 systems stored in an innovative database linked to other sources of biological and experimental data.

NERSC: in-house simulation software, *in lucem molecular mechanics* (ilmm) on Franklin & Hopper

V. Daggett (U of Washington)



Left: Dynameomics journal cover story; article explained how the database can be mined to obtain insight into a variety of biologically relevant questions. Right: computed structure of a thermophilic enzyme showing why it retains its native conformation at high temperatures to a much greater degree than do other proteins.

Structure 18 (4) April 2010; Protein Engineering Design and Selection 2010 23(5):327-336

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FLASH Can Model Laser-Created Dense Plasmas

Objective: Modeling the shockwave physics observed in laboratory laser experiments.

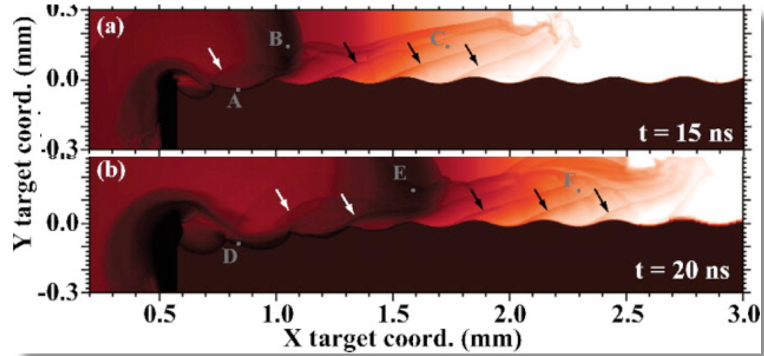
Implications: High-energy laser facilities create hydrodynamic conditions relevant to astrophysics, specifically Supernova explosions.

Accomplishments: Simulations using the FLASH code reproduce most experiment features but certain aspects differ in ways that are not completely understood.

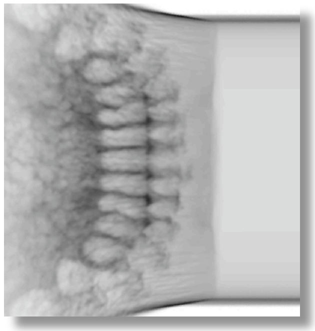
- May be due to magnetic fields that are not currently considered in such simulations.
- Differences in Equation of State and 2-D vs. 3-D structure also examined as important effects.

NERSC: FLASH runs (64 - 2,048 cores) and visualization using VisIt (64 - 128 cores) on Franklin; movies generated on DaVinci

T. Plewa (FSU)
P. Drake (UMich)



2-D FLASH *simulations showing development of high- (black arrows) and low-Mach (white arrows) shock waves in a Nike laser experiment.*



Results from 3-D FLASH simulation observing a blast-wave-driven Rayleigh Taylor instability induced by the Omega Laser. The experiment was designed to be well scaled to conditions in the outer layers of Supernovae.

PHYSICS OF PLASMAS 17, 056310 (2010)
PHYSICS OF PLASMAS 17, 052709 (2010)

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

Accelerator Simulations "Reframed"

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

W. Mori (UCLA)

Objective: Use advanced simulation tools to study feasibility, and optimize conceptual design, of plasma-based linear colliders.

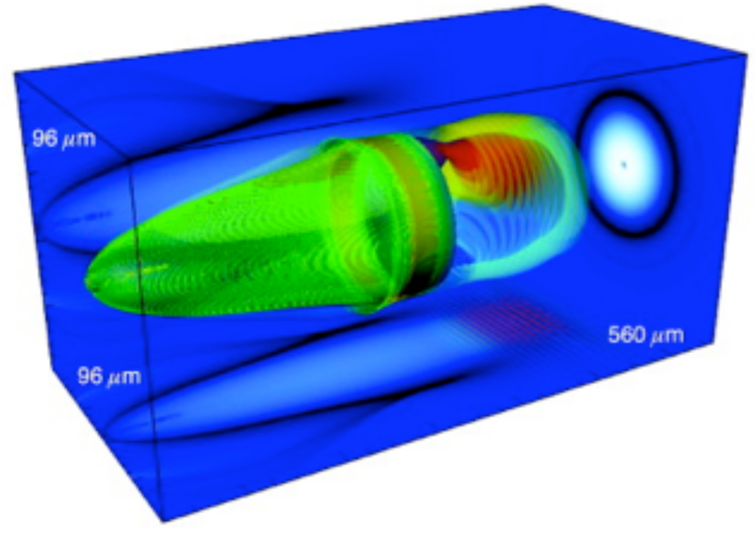
Implications: Development of acceleration methods more than 1,000 times greater than conventional technology.

Accomplishments: Developed a new Lorentz frame simulation method.

- Minimizes disparity in scales between the laser and plasma, thus reducing the number of required time steps.
- Simulations run 20-300X faster.

NERSC: Uses OSIRIS code on Franklin; scales to more than to 16,000 cores.

- NERSC resources + INCITE used to develop method and code; runs now on BG, XT5, elsewhere.



Simulation results in the boosted frame for a 1.5-GeV self-injected electron beam in a single-stage laser-wakefield accelerator. The laser propagates from left to right and drives the wakefield that traps and accelerates electrons (green isosurfaces and blue projections).

Nature Physics 6, 311 - 316 (2010)
Computer Physics Communications 181, 869-875 (2010)

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MADmap Cosmic Microwave Background Analysis Software Scales

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: **Analyze the Planck Cosmic Microwave Background (CMB) satellite data. Planck will scan the entire sky for 2.5 years.**

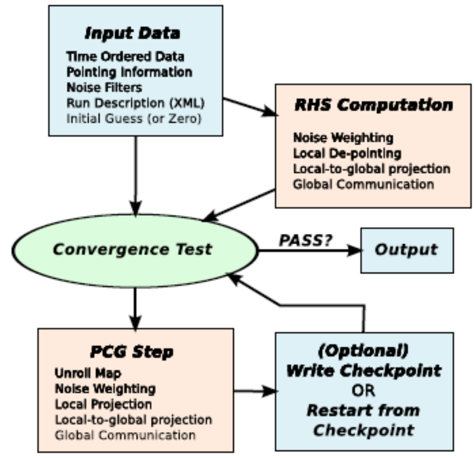
Implications: **CMB is the most valuable resource for understanding fundamental physics and the origins of the universe.**

Accomplishments: **MADmap software developed and extensively tested against simulated time-ordered data that include realistic instrument systematics.**

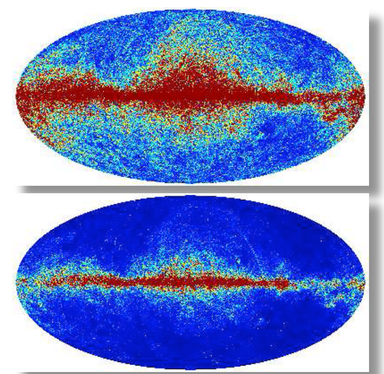
- **Scales to ~10^{11} time samples, ~10^{8} pixels and ~10^{4} processor cores**
- **NASA Public Service Award in 2010**

NERSC: **CMB-NERSC collaboration dates to ~1997, involves extensive I/O improvement and benchmarking, lately Franklin/NGF/DVS tuning; also, extensive use of 256-core Planck Cluster; NGF is a key resource – allows production on Franklin/Hopper, analysis on Planck.**

Cantaloupo, Borrill, Jaffe, Kisner, Stompor, others



Graphical overview of the mapping process. Blue boxes represent data products, pink boxes represent computational procedures, and RHS is the "right hand side" calculation.



Two polarization vector maps made from simulated time-ordered data

The Astrophysical Journal Suppl Ser, Vol 187, No 1,March 2010
Astronomy & Astrophysics, Vol 493, 753–783 (2009)

ENERGY | Office of Science | HEP

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Simulation Can Explain – *and Help Avoid* – Radiation Damage in Ceramics

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

Objective: Simulation aimed at atomic-level understanding of structural defects in materials subjected to extreme conditions.

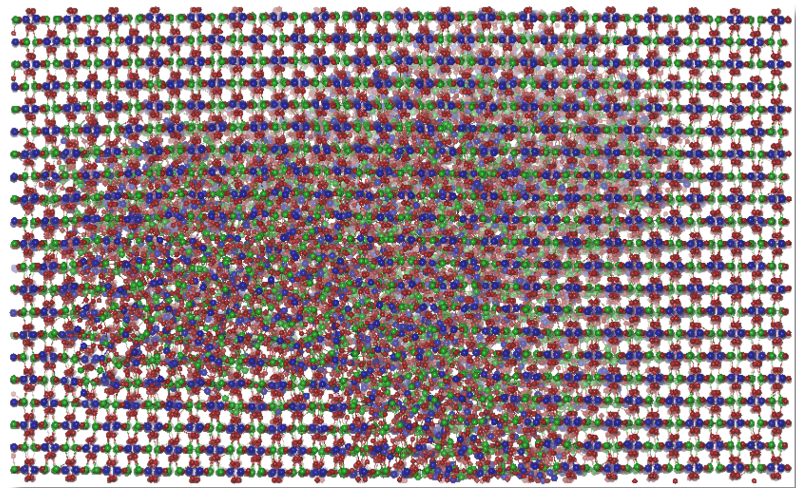
Implications: Radiation tolerant ceramics are needed for nuclear waste immobilization. This work examined processes that can result in degradation of thermo-mechanical properties and reduced chemical durability.

Accomplishments: Simulations have shed light on radiation damage and defect accumulation in silicon carbide, zircon, zirconia, uranium dioxide and pyrochlores.

- Identified amorphization mechanisms.
- Demonstrated that ceramics can be designed to dissipate radiation damage or self anneal leaving the material undamaged.

NERSC: Used *DL_POLY* code on Franklin, Jacquard, 256-512 cores

R. Devanathan (PNNL)



Result of a molecular dynamics simulation of Zircon ($ZrSiO_4$) showing damage to the crystal lattice as a result of high-energy uranium recoil. The simulation revealed the occurrence of direct-impact amorphization of this otherwise durable mineral.

Review Article in Nuclear Instruments and Methods in Physics Research B 267 (2009) 3017–3021

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

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Studies May Allow "Tuning" of Transparent Conducting Oxides (TCOs) for Energy Applications

Objective: Thorough understanding of novel metal oxides via systematic *ab initio* electronic structure studies.

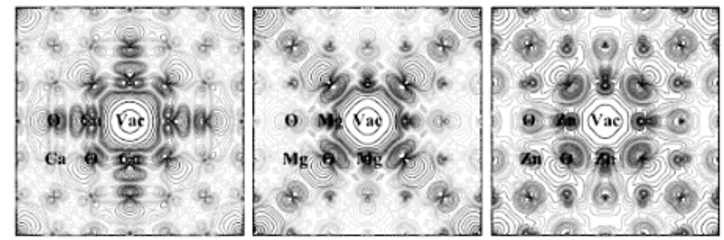
Implications: These materials have applications in photovoltaic cells, flat panel displays, and flexible & invisible electronics but optimal performance is a challenge because of optical / electronic tradeoffs.

Accomplishments: Discovered that several unique TCO properties arise from certain types of strong metal-oxygen bonds.

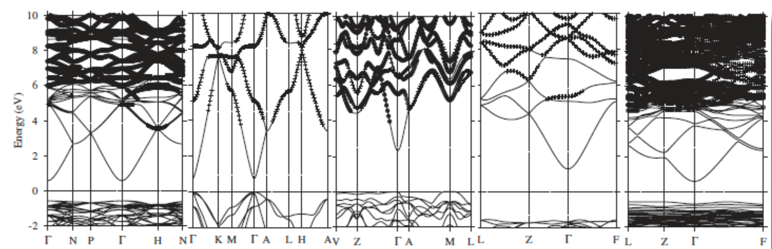
- Explained differing conductivity of oxygen deficient and doped oxides; due to crystal symmetry & coordination geometry effects.
- Suggested how doping may allow "tuning" of electronic and optical properties.

NERSC: Requires custom code, more time-consuming than VASP; 1-4k Franklin cores

J. Medvedeva (Missouri U of Sci & Tech)



Contour plots of electron density in three metal oxides (calcium, magnesium and zinc).



Calculated electronic band structure for five undoped metal oxides. Medvedeva's work shows that multicomponent oxides may offer a way to overcome the electron localization bottleneck that limits charge transport in wide band-gap main-group metal oxides.

Phys. Rev. B 81, 125116 2010 &
Book Chapter, Transparent Electronics: From Synthesis to Applications, Eds. A. Facchetti and T. Marks, John Wiley & Sons, April 2010

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Molecular Dynamics Can Predict Continuum-Scale Porous Media Properties

NERSC
NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

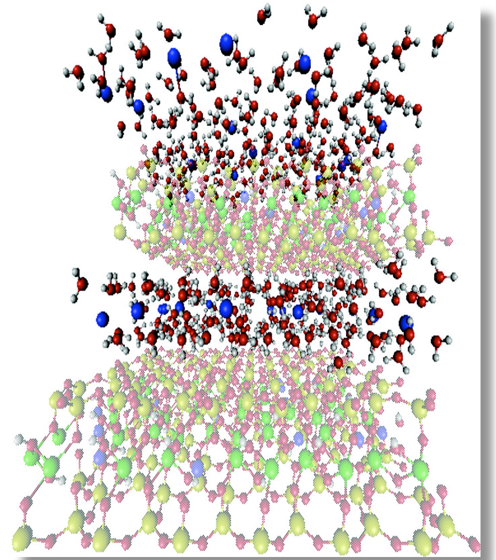
Objective: ***Molecular-scale*** **understanding of chemistry and mass transport in nanoporous geologic media.**

Implications: **Nanoconfined water & solutes behave differently than their bulk liquid counterparts; difference may result in nanoporous media with remarkable properties for contaminant remediation, nanofluidics, and biotechnology.**

- ***Accomplishments:*** **Showed that molecular simulations at nanometer- and nanosecond-scale can help explain behavior of natural porous systems on scales of centimeters and days.**
- **Can accurately predict diffusion coefficients widely used in evaluating radioactive waste and CO_2 repositories.**

NERSC: **Used MOLDY code, 32 -64 cores on Bassi**

I. Bourg, G. Sposito (LBNL)



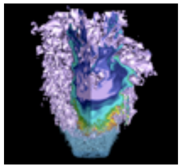
Snapshot of the molecular dynamics simulation cell for the two-layer hydrate of Na-montmorillonite, with Na (blue), water O (red), and water H (white) atoms in the interlayer and Si (yellow), Al (green), Mg (blue), O (red), and H (white) atoms in a clay mineral structure.

Environ. Sci. Technol. 2010, 44, 2085-2091

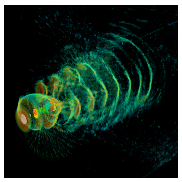
U.S. DEPARTMENT OF ENERGY | Office of Science | BES

BERKELEY LAB

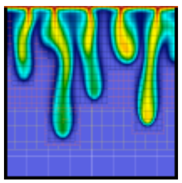
About the Cover



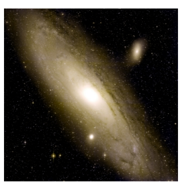
Low swirl burner combustion simulation. Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodiffusively unstable fuel. Simulated using an adaptive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



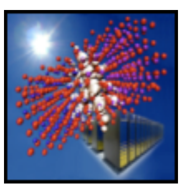
Hydrogen plasma density wake produced by an intense, right-to-left laser pulse. Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour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



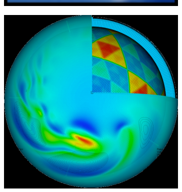
Numerical study of density driven flow for CO_2 storage in saline aquifers. Snapshot of CO_2 concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO_2 is converted into negatively buoyant aqueous phase, thereby improving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