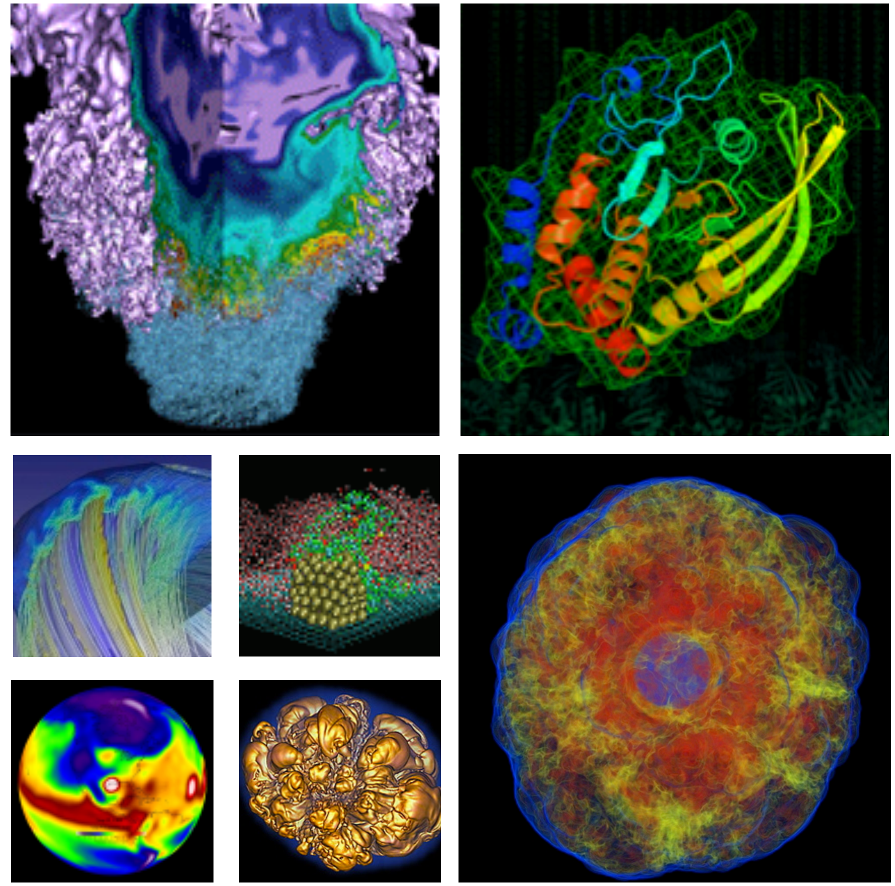
NERSC Science Highlights



NERSC

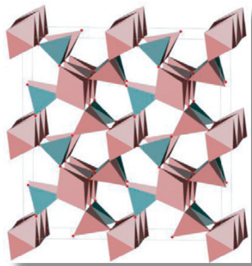
Selected User Accomplishments

January 2013

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

NERSC User Science Highlights

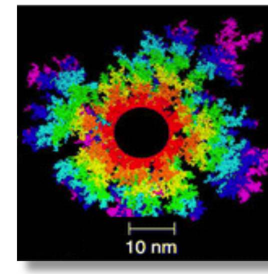


Materials

ab initio study of key ceramic structure is important first step in understanding advanced properties of important mineral
(W-Y. Ching, UMKC)

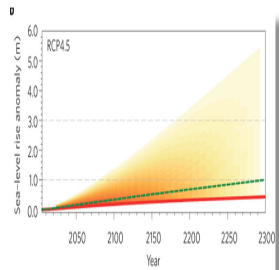
Chemistry

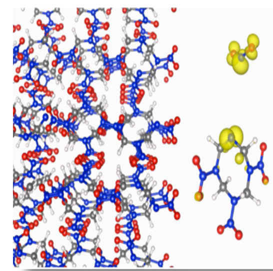
New method affords molecular-level insight into process responsible for lithium battery failure
(T. Miller, Caltech)



Climate

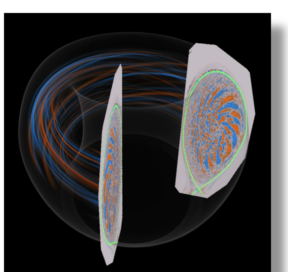
Study sheds light on question of how well climate change mitigation might defer sea level rise
(A. Hu, NCAR)





Materials

Computation helps elucidate mechanism of explosive decomposition
(M. Kuklja, U. Maryland)

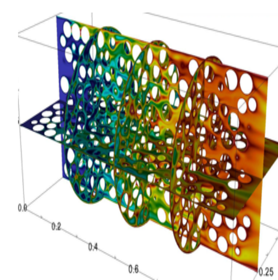


Fusion

Explanation of the source of intrinsic rotation in fusion plasmas may be key finding for ITER device
(C.S. Chang, PPPL)

Math

AMR method allows pore-scale modeling of carbon sequestration effects at unprecedented scale
(D. Trebotich, LBNL)



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Nailing Down the Structure of Mullite

NERSC

- **Mullites (minerals containing aluminum, silicon, and oxygen in varying proportions) are strong candidates for advanced structural, optical, and ceramic applications**
- **Electronic structure has never been studied**
- **This work: mechanical, optical, electronic, and elastic properties from first-principles modeling; used NERSC-supplied software**
- **Covered an entire range of Mullites despite significant challenge in accounting for varying mineral content**
- **Results: fundamental explanation of experimentally observed structure and properties of mullite phases as a function of their composition**

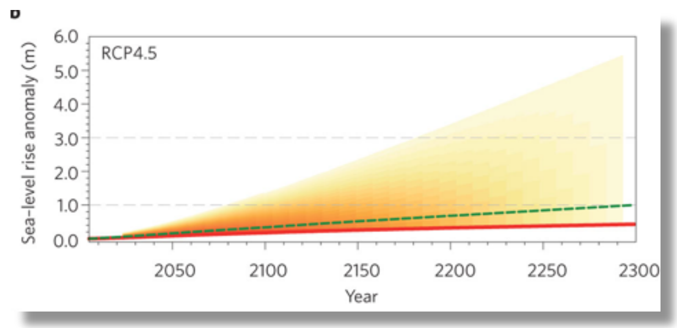
On the Cover: September issue of the Journal of the American Ceramic Society featuring Prof. Ching's simulations

J. Am. Ceram. Soc, 95 [7] 2075–2088 (2012)

Climate Change Mitigation and Sea Level Rise

- Perception is that climate change mitigation will significantly reduce rate of sea level rise

- Goal: Calculate full ocean heat content, total sea level rise due to thermal expansion and contributions from glaciers and ice sheets with varying levels of mitigation.
- CCSM4 scenario analysis covering the years 2000 – 2300
- Showed that with aggressive mitigation, temperatures could stabilize
- But sea-level rise (SLR) will continue for next few hundred years
- With no mitigation SLR will continue basically unabated for centuries.
- Highlighted at BER Advisory Council meeting, June 2012



Calculated globally averaged sea-level rise anomaly (rel. to 1986-2005) due to thermal expansion (red line) and total (green). Shading indicates uncertainty (lighter means less certain)

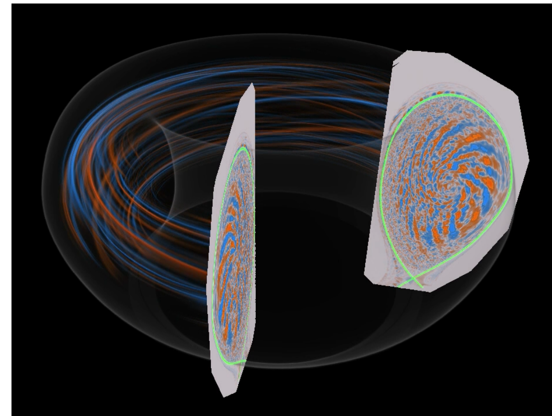
Nature Climate Change, 2, 576-580

BER

W. Washington, G. Meehl, A. Hu (NCAR)

Science at Scale: Plasma Finding is Key for ITER

- **Understanding intrinsic toroidal rotation of tokomac plasmas is key for successful performance of future fusion devices.**
- **Used SciDAC XGC1 gyrokinetic code to model relevant multi-scale physics over the entire plasma volume of the DIII-D fusion reactor, explaining the intrinsic rotation phenomenon**
- **ITER could achieve adequate spin up using this understanding.**
- **Such multi-physics simulations are possible only on Petascale HPC — will require Exascale in the future.**
- **Findings point to the plasma edge as a source of rotation and the turbulence as a vehicle for inward propagation.**
- **10-M hour simulation using 1/2 of Hopper**



Simulations at NERSC using the XGC1 gyrokinetic cod helps us to understand the mechanism of the intrinsic rotation in self-regulating plasmas, and gives important information about the prediction and operation of the self-regulation plasmas in ITER and other future fusion reactors.

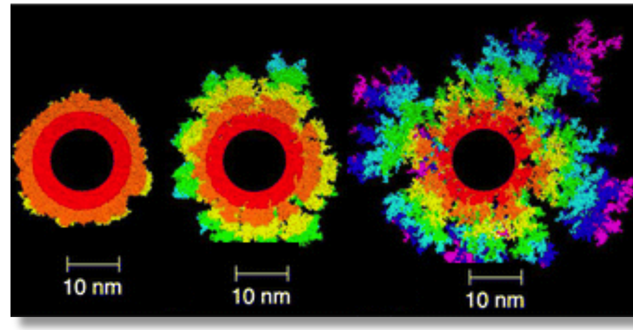
Nucl. Fusion 52 (2012) 063013

Understanding Battery Failure

- **Motivation: solid "dendrite" deposits that form during recharging are a major source of failure in lithium-ion batteries**
  - Mitigation is an important industrial challenge
  - Detailed molecular mechanism poorly understood

- **Approach: use a new "coarse-graining" method (introduced by Prof. Miller's group) that enables battery electrode simulation across the long time and length scales associated with charging and discharging**

- **Accomplishment: direct simulation of electrochemical deposition, revealing the molecular mechanisms governing dendrite growth.**
  - Showed how certain kinds of electric pulses during charging can suppress dendrite formation



Simulation showing dendrite forming in a lithium battery. This work provides a molecular basis for designing charging methods that mitigate dendrite formation while minimally affecting battery charging times. "NERSC resources were the primary driving force in making this research possible." – Tom Miller

THE JOURNAL OF PHYSICAL CHEMISTRY C

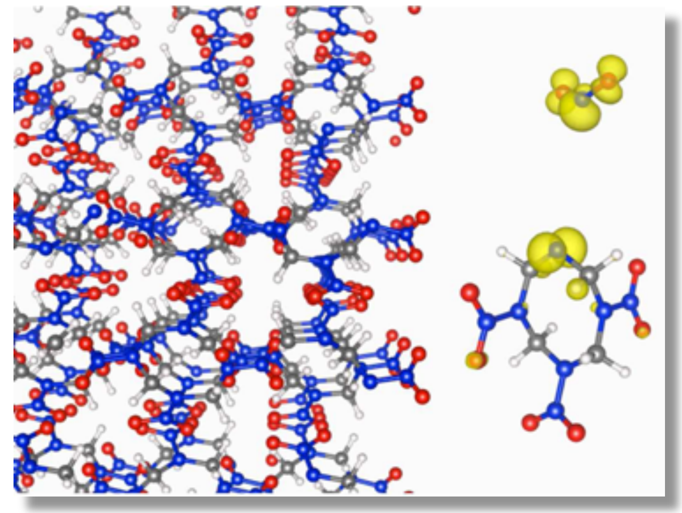
Vol 116 (50) November 19, 2012

BES

PI: T. Miller, (Caltech)

Computational Studies Shed Light on Energetic Materials Degradation

- **New theoretical study is important for fuels, propellants, and explosives**
- **Fundamental knowledge about the relationship between chemical structure and initiation of rapid energy release in explosives is lacking.**
  - Needed to help avoid accidental detonation
- **Quantum simulations using NERSC-provided software examined the decomposition of HMX, a famous explosive.**
- **HMX has been extensively studied, but this work is the first to provide detailed insight into how a material's decomposition mechanism relates to morphology of its crystals, including surfaces, defects, and particle size.**
- **Used a new, coupled theory approach that yielded results not attainable from any experiment.**



Crystal structure of HMX, a powerful but relatively insensitive high explosive. A new computational strategy developed by NERSC researchers may help scientists better control fast, highly energetic chemical reactions.

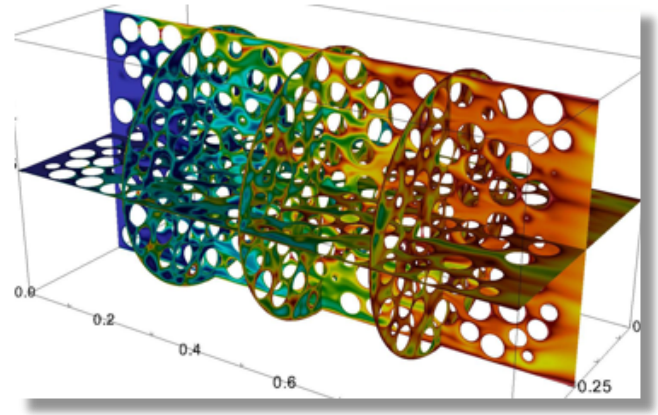
JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

June 15, 2012

Onise Sharia, Maija M. Kuklja (University of Maryland)

Science at Scale: Understanding CO_2 Sequestration

- **Goal: simulate "far-from-equilibrium" conditions in flow, transport, and reaction coupling for subsurface CO2 injection.**
- **Approach: combine adaptive mesh refinement CFD methods with complex geochemistry to provide direct pore-scale modeling of multicomponent reactive transport**
- **New insights into pore scale dynamics will greatly improve our ability to develop scientifically defensible predictive models.**
- **Simulated the largest pore-scale problem ever attempted, with flow in a capillary tube packed with crushed calcite: 1.6-billion grid points, using over 100,000 cores on Hopper.**
- **Grid resolution is now very close to that of imaging experiments, enabling a key EFRC goal of combining simulation and experiment.**



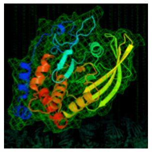
Calculated calcium concentration in a large capillary tube capturing pore-scale behavior.

2012 NERSC NISE Allocation

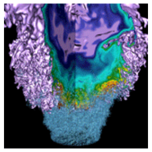
Center for Nanoscale Control of Geologic CO2

Water Resources Research, Vol. 48, W03527, 2012

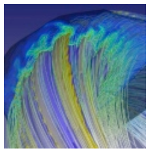
About the Title Slide Images



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)

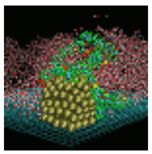


Detailed structure of a flame from a Low swirl burner combustion simulation. Image courtesy of John Bell, LBNL.

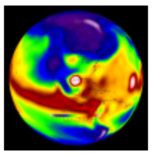


Representation of a plasma from a magnetic fusion energy simulation. Magnetic fields within the plasma are represented as white lines and the temperature is shown as blue/yellow surface (Linda Sugiyama, MIT)

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)

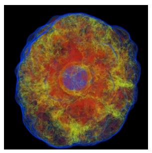


Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

National Energy Research Scientific Computing Center