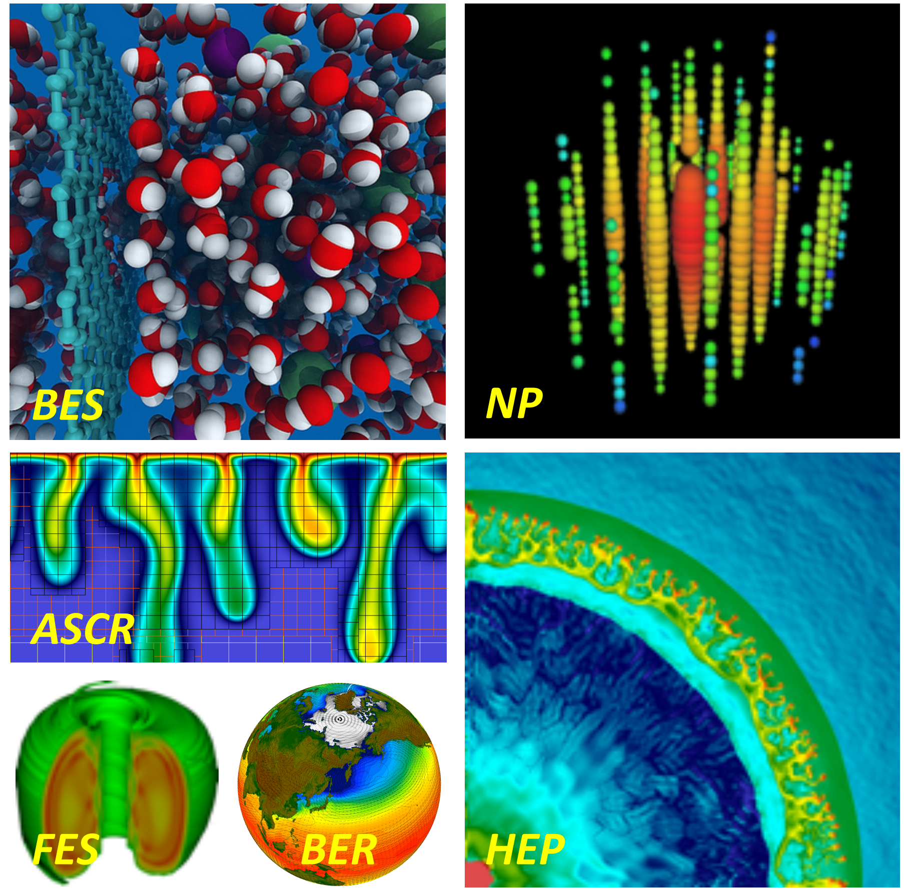
NERSC Science Highlights



NERSC 40 YEARS at the FOREFRONT 1974-2014

Selected User Accomplishments

June 2014

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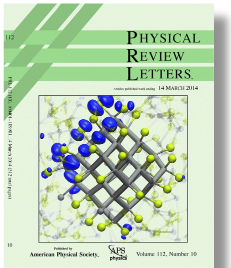
NERSC User Science Highlights



Materials

New models and methods suggest promising approach to solar energy conversion

(G. Galli, UC Davis)

Climate Modeling

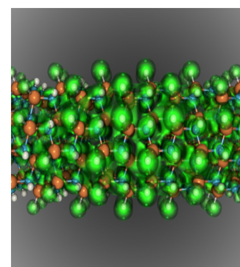
Study suggests reduced river flooding as a result of greenhouse gas-induced warming

D. Stone (LBNL)

Chemistry

Study explains, for the first time, chemical stabilization of metal complexes in water

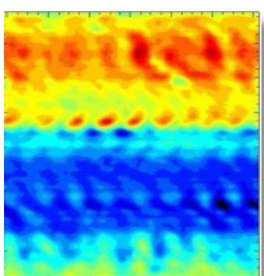
(S. Xantheus, PNNL)



Energy

Simulations using a NERSC-provided method suggest how to improve LED efficiency

(E. Kioupakis, U Michigan



Fusion

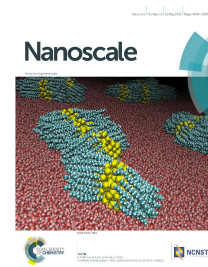
Edison helps calm the stormy seas of a tokamak plasma

(J. Citrin, Dutch Institute for Fundamental Energy Research)

Materials

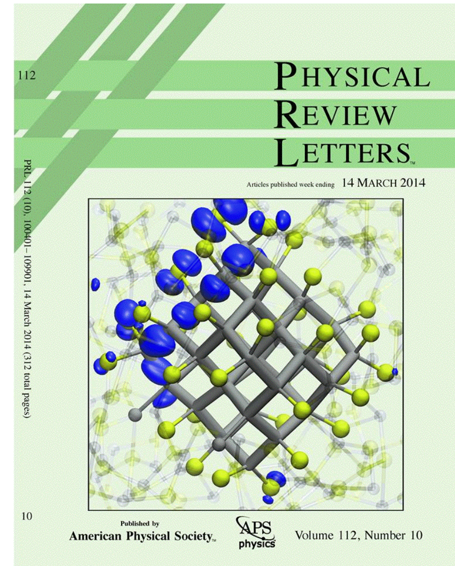
Modeling helps explain self-assembly and aggregation of coated nanoparticles

(G. Grest, SNL)



Promising Approach to Solar Conversion

- **Important new result in search for materials that can “harvest” (i.e., create energy from) sunlight**
- **Approach: study silicon nanoparticles embedded in earth-abundant, non-toxic zinc-sulfur materials and show how to design such materials optimized for solar absorption**
- **Required creating realistic models of the new materials as well as improved scalable computational methods to evaluate them**
- **Results from *ab initio* simulations at NERSC show how the sulfur atoms enhance solar energy conversion by lowering the band gap and enhancing charge mobility.**



On the Cover: Computed electron density in a hypothetical ZnS matrix containing silicon nanoparticles showing how the sulfur atom lone pair electrons (blue) form complementary charge transport channels for electrons and holes, resulting in a lower electronic band gap

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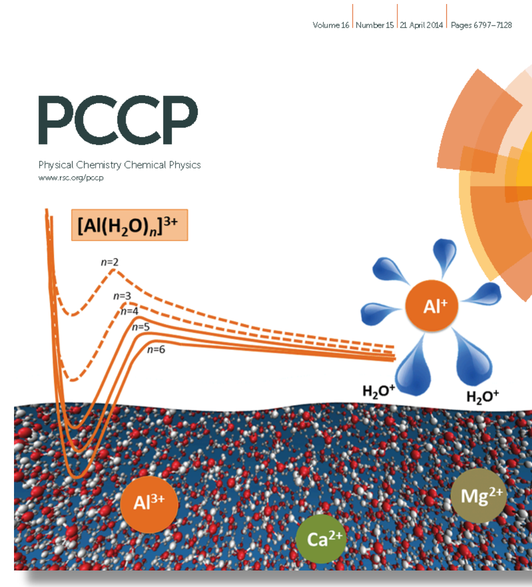
G. Galli (UC Davis) ***Physical Review Letters, 112, 106801 (2014)***

Basic Understanding of Water as Solvent

- **Understanding how metal atoms dissolve in water is of importance in many chemical and biological processes related to energy, catalysis and environmental remediation.**
- **Metal ions in water usually have large atomic charges but precisely how these ions are stabilized as metals dissolve is unclear.**
- **This study elucidated the mechanism behind the stabilization of multi-charged aluminum, calcium, and magnesium ions via a detailed theoretical analysis.**
- **The results quantify for the first time how binding between metal ions and water is aided by simultaneous minimization of the repulsion between the water molecules.**

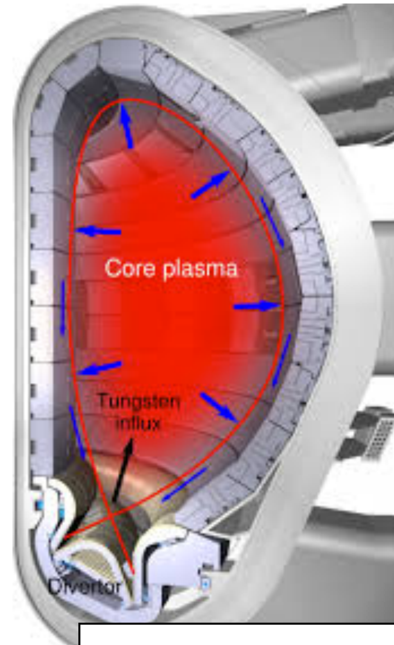


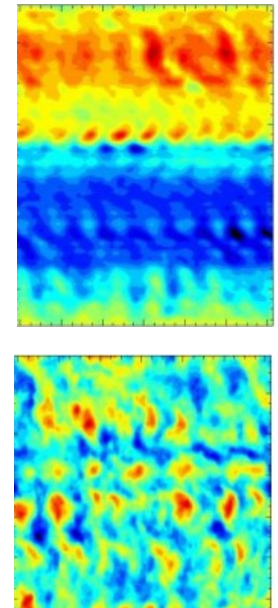
On the Cover: This composite artist concept includes computed potential energy curves for the approach of up to six water molecules to form a hydrated aluminum cluster. The curves' visual simplicity belies the significant computational complexity involved at the level of theory used in this study.

Physical Chemistry Chemical Physics Volume 16 Number 15 21 (April 2014)

Tokamak Stabilization via Simulation

- Simulations show how overcoming ion instabilities in hot plasma can boost a fusion reactor's energy output.
- Sheds light on how fast ions in the plasma affect microturbulence
- Matched findings obtained using the Joint European Torus tokamak but also apply to ITER
- Excellent example of experiments forcing an extensive direct numerical simulation validation effort
- Edison's improved compute speed played a key role; allowed inclusion of magnetic fluctuations and additional ion species, which led to less turbulence





Left: Side view of a tokamak plasma. Right: Results from a gyrokinetic plasma simulation done at NERSC with fast ions (top) and without (bottom), showing how microinstabilities driven by large gradients in temperature and density can limit fusion output.

Physical Review Letters, 111, 155011 (2013)

Unusual Climate Modeling Result: Decreased Flooding From Higher Temps

- **Results from a groundbreaking study suggest that greenhouse gas-caused climate change substantially *reduced* chances of flooding in the Okavango River Basin, an ecologically/geographically unique region in southern Africa.**
- **The counterintuitive simulation result is because with warmer air, the river takes longer to flow to the delta with more evaporation and less flooding.**
- **The huge flooding observed recently in this area would apparently have been much *worse* without a warmer climate.**

The inset shows the region subjected to intense flooding in recent years. Climate simulations done at NERSC strongly suggest that this flooding is not a result of greenhouse gas-induced climate change.

Journal of Hydrology 511 (2014) 350–358

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D. Stone (LBNL)

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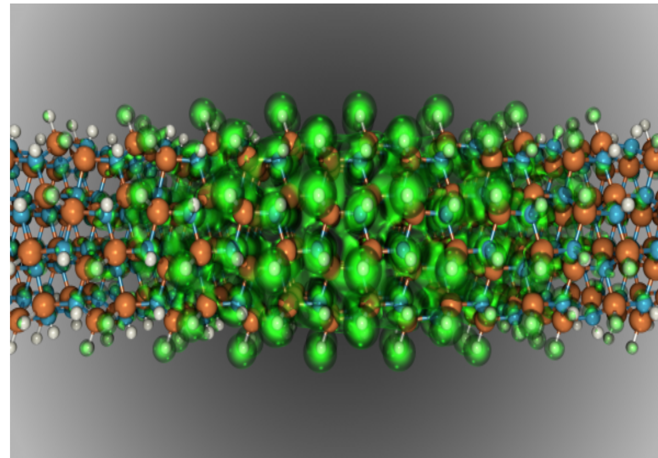
Improving LED Efficiency Through Computation

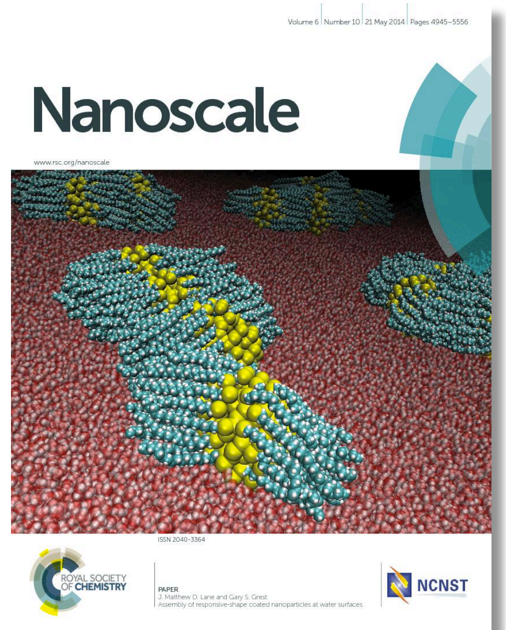
- **Simulations at NERSC have shown that semiconductors made of oft-used materials sized with ultra-thin dimensions could lead to dramatically improved LED efficiency.**
- **The study showed how nanoscale wires exhibit a "quantum confinement" effect that causes emission of green light at high efficiency. Today's commercial LEDs using the same material emit at lower efficiency.**
- **The work required the BerkeleyGW software provided by NERSC consultant Jack Deslippe. The GW method is at the leading edge of computational materials science research because it can accurately model how light interacts with matter in semiconductors, power amplifiers, and other devices.**



On the Cover: This image, prepared by NERSC visualization expert Burlen Loring, will appear on the cover of the American Chemical Society journal **Nano Letters** ***in July, 2014. It shows electron distribution from a simulation of a nitride nanowire. "Semiconductor Today" also ran a story on the results because the work could lead to LED efficiency improvements in portions of the spectrum where efficiency in traditional LEDs is known to fall.***

Controlling NanoParticle Assembly

- **Soft materials consisting of polymer-coated nanoparticles (NP) can be used for photonics, filtration, photovoltaics, and other important applications.**
- **However, use is limited by ability to control NP assembly into ordered structures.**
- **This is work used molecular dynamics to model self-assembly and aggregation of coated NPs at a water-vapor interface.**
- **Surprisingly simple short chain polymer coatings can effectively be used to selectively control aggregation of very small nanoparticles.**
- **Modeling in this way allows fine tuning of assembled NP structure by varying polymer composition but requires very long simulations.**



On the Cover: Yellow spheres are gold nanoparticles, the alkane chains (coatings) are in blue/white, and water in red/white. Some chains are terminated with COOH (polar), others with CH3 (non-polar), which determines their affinity for the surrounding water.

PI: G. Grest (SNL)

Nanoscale, 2014, 6, 5132

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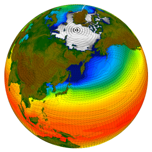
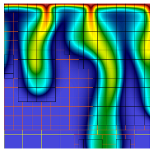
About the Title Slide Images

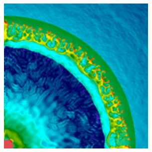
Evolution of electrical current density, parallel to magnetic field, in the Pegasus Toroidal Experiment; provided by John O'Bryan and Carl Sovinec, University of Wisconsin-Madison; Sponsored by Office of Fusion Energy Sciences



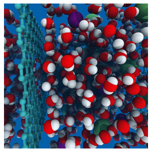
A single month from a simulation of the 20th century by the CCSM capturing wind directions, ocean surface temperatures, and sea ice concentrations. Image courtesy Gary Strand (NCAR) and copyright University Corporation for Atmospheric Research. Sponsored by Office of Biological and Environmental Research



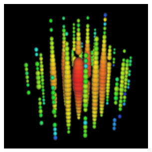
Simulation of density-driven flow for CO_2 storage in saline aquifers. Shown is a snapshot of the CO_2 concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Sponsored by Office of Advanced Scientific Computing Research.



Collision between two shells of matter ejected by a massive star in two pair-instability supernova eruptions, only years apart, just before the star dies, showing a slice through a corner of the event. Shell radius (red knots) is about 500 times the Earth-Sun distance. Colors represent gas density (red is highest, dark blue is lowest). Image courtesy of Ke-Jung Chen, School of Physics and Astronomy, Univ. Minnesota. Sponsored by Office of High Energy Physics.



Snapshot from a Molecular Dynamics simulation showing water molecules (red and white), and sodium, chloride ions (green and purple) in saltwater, encountering a sheet of graphene (pale blue, center) perforated by holes of the right size, with water passing through (left side), but sodium and chloride being blocked. Provided by D. Cohen-Tanugi and J. C. Grossman, MIT; Sponsored by Office of Basic Energy Sciences



Observation of a PeV-energy neutrino. Each sphere represents a digital optical module sensor in the IceCube detector. Sphere size is a measure of the recorded number of photoelectrons. Colors represent arrival times of photons (red, early; blue, late). Sponsored by Office of Nuclear Physics

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