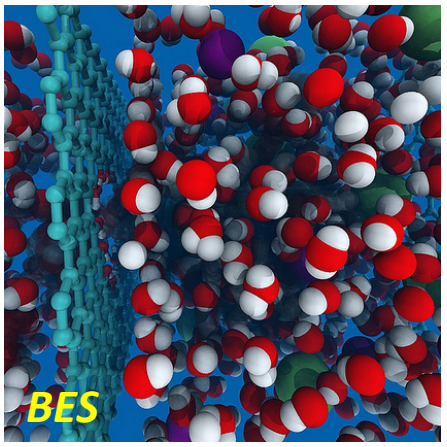
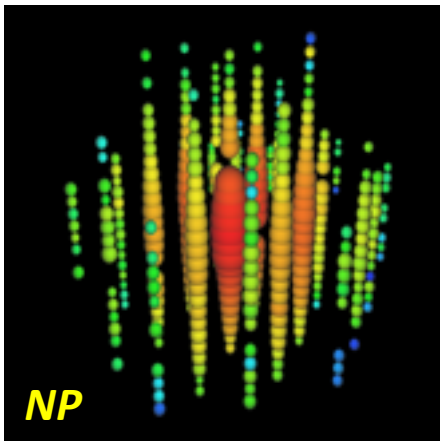
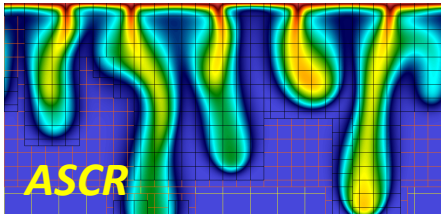
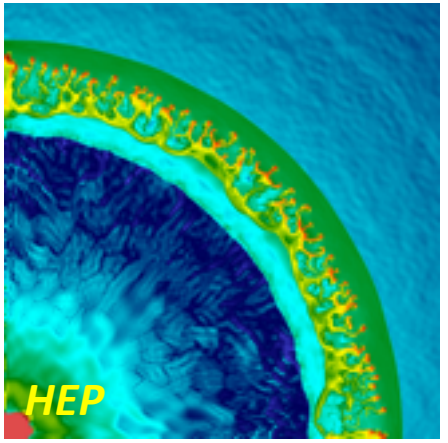
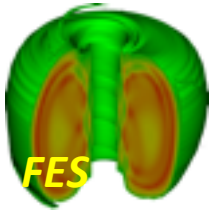
# NERSC Science Highlights

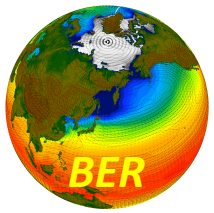



NERSC 40 YEARS at the FOREFRONT 1974-2014

## Selected User Accomplishments

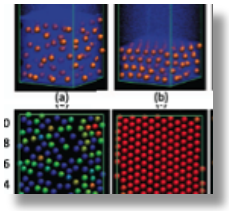
### March 2014

U.S. DEPARTMENT OF ENERGY | Office of Science



BERKELEY LAB
Lawrence Berkeley National Laboratory

# NERSC User Science Highlights



## Materials

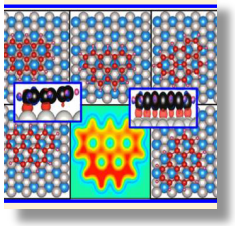
Seven different ALCC-allocated simulation studies show how controlling nanoparticle interaction might produce new materials
**(G. Grest, Sandia)**

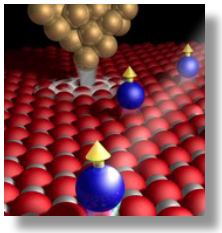
## Energy

Computation suggests an approach to improving battery performance using materials that had previously been disregarded
**(G. Cedar, MIT)**

## Chemistry

Study of Olympics-inspired molecule provides insight into design of improved electronic devices.
**(A. Kara, U. Central Florida)**





## Physics

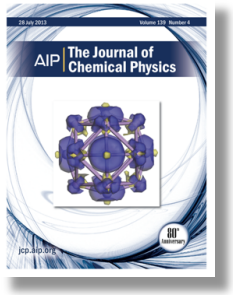
Combined theoretical/ experimental study explores magnetism of a single atom
**(S. Gangopadhyay, IBM)**


## Geoscience

Materials informatics helps optimize gas storage
**(B. Smit, UC Berkeley)**

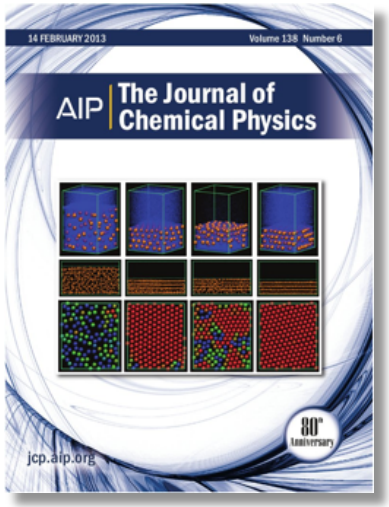
## Materials

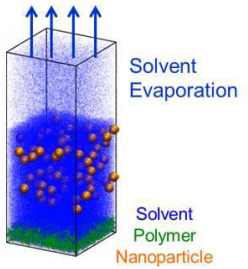
Study suggests a route to new metallic structures having huge but tailored magnetic characteristics
**P. Jena (VCU)**



# Controlling Nanoparticle Interactions to Engineer New Materials

- **Goal: Use simulation to better control self-assembly of nanoparticles to form new devices**
- **Completed: Seven major simulation studies, including a study of diffusion in weakly interacting polymers that have nanoparticles dispersed in them; results conclusively show two very different classes of behavior depending on nanoparticle size.**
- **Molecular dynamics simulations of nanoparticle assembly during controlled liquid evaporation show that quality of the nanoparticle crystal formation is a function of evaporation rate.**



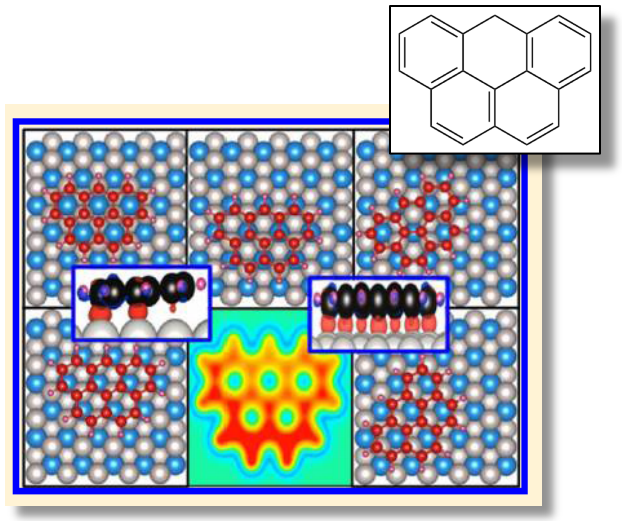




***On the Cover:** Snapshots from a simulation of solvent evaporation; solvent shown in blue; time increasing from l to r; top is side view, bottom is top view.*

***Journal of Chemical Physics, February 8, 2013***

# Computational High-Throughput Screening of Organic Materials for Solar Energy and Lighting

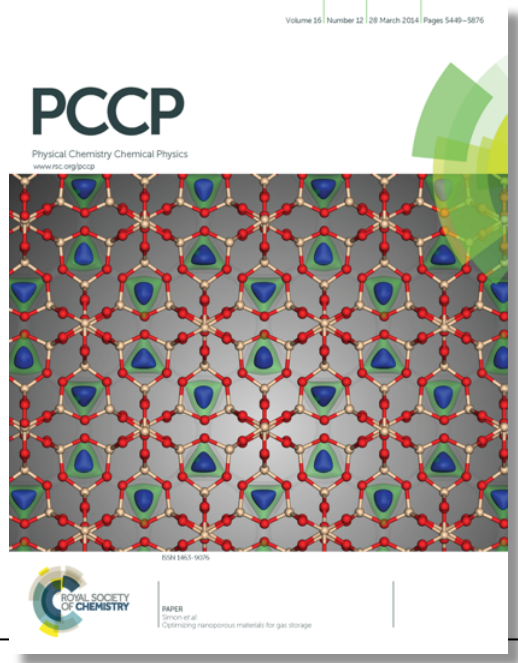
- **Goal: Explain the electronic structure of the interface between organic molecules and metal surfaces to help design light-weight, flexible, low-cost, and durable electronic devices.**
- **Completed: Studied adsorption of the "Olympicene" molecule on copper to explain characteristics of metal-to-carbon bonding that takes place – bonding that represents a unique transition between physical adhesion and true chemical bonding.**
- **Three papers already published; five will be submitted within the next few months.**



***Olympicene is an organic molecule consisting of five fused rings in the shape of the Olympics emblem that has promising electronic and optical properties. The image shows various views from a simulation study of the molecule adsorbed on a surface of copper atoms.***

# Materials Informatics Helps Optimize Gas Storage

- This work created an efficient way to computationally screen over 136,000 hypothetical and 187 known materials to investigate what properties lead to high capacity for methane storage.
- Important, because better storage mechanisms are needed for methane to become an economically viable alternative fuel.
- High-throughput analysis of thermodynamic factors showed how effectiveness of gas absorption depends on the structure of the material pores.
- Because these porous materials have highly tunable structures, the results can help guide future designs.

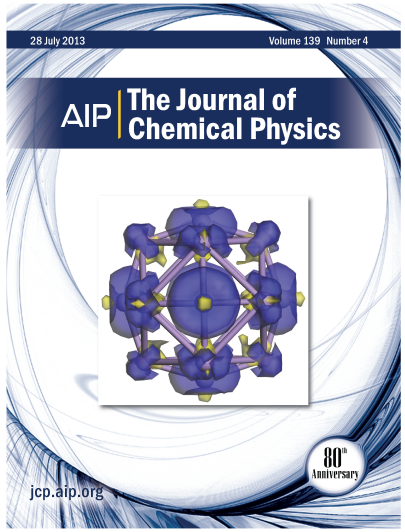



*On the Cover: This alluring visualization shows the crystal structure (red, tan) and calculated energy landscape (blue, green) of a top-performing gas storage material based on screening and simulation done at NERSC.*

***Phys.Chem.Chem.Phys.,*** 2014, 16, 5499

# Colossal Magnetic Moments Discovered

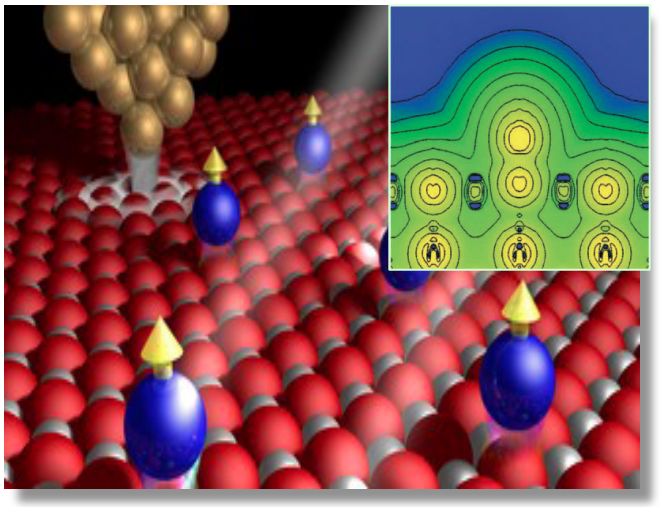
- Computation has suggested the possibility of creating large, hollow cage molecules that could have unique, tailor-made magnetic properties.
- Studies at NERSC show that stable, hollow atomic cages larger than even $C_{60}$ ("fullerene") are possible, providing a route to the synthesis of atomic clusters that can act as molecular magnets.
- Such clusters, with their huge magnetic strength, may have application in future "spin-based" microelectronic devices, possibly creating a new generation of super-fast, energy-efficient computers.




*On the Cover: An image showing the computed electronic spin deformation density in a hypothetical atomic cluster consisting of 12 manganese and 6 carbon atoms. The NERSC study suggests that this new kind of metal will be stable and have a huge magnetic strength.*

# Exploring Magnetism in a Single Atom

- A combined theoretical/experimental study has shown, for the first time, remarkable magnetization effects in a single cobalt atom.
- This fundamental result may have great implications for future magnetic devices like hard drives, molecular magnets, computer memories, and quantum computers.
- Computation was important in revealing the physical & electronic structure of the cobalt atom and in explaining how its magnetic properties depend on its electron orientation.
- As the dimensions of a magnetic "bit" shrink to atomic scales, quantum mechanical effects can greatly affect the magnetization. This study revealed the limit of how much magnetic energy can be stored in an atom.

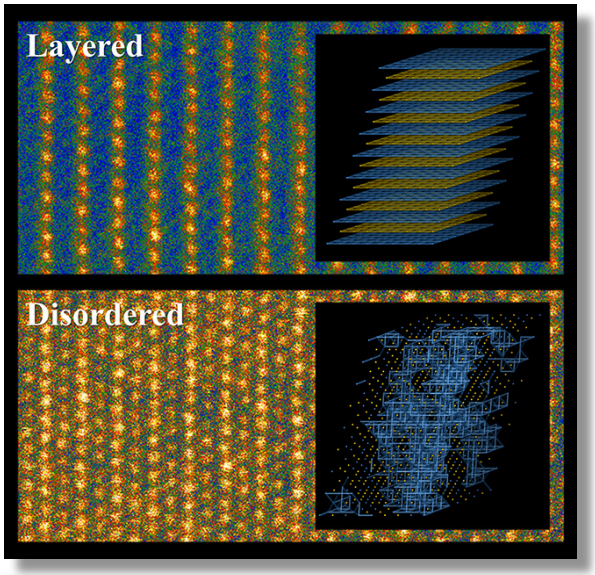


*A conceptual image showing a microscope tip (gold) used to probe the quantum spin state behavior of individual cobalt atoms (blue) on a red MgO surface. Image © 2014 EPFL. The insert at top-right shows calculated valence electron charge density of one Co atom from computation done at NERSC.*

*Science 30 MAY 2014 • VOL 344 ISSUE 6187*

# Disordered Materials Hold Promise for Better Batteries

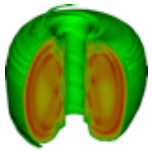
- Computation at NERSC has suggested a new route to high energy density cathodes for rechargeable lithium batteries.
- The new cathodes use disordered materials that had generally been considered unsuitable for batteries.
- Density functional theory (DFT) simulations explained the high capacity of the disordered material during battery charge/discharge cycles by showing how lithium ions could easily percolation through certain channels that are active in disordered structures.
- The work also suggested why disorder has not been pursued as a strategy before, pointing to an exciting new class of energy materials.



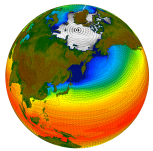

*Conventional ordered lithium cathode material (top) and the new disordered material studied by researchers at MIT (bottom) as seen through a scanning transmission electron microscope. Inset images show diagrams of the different structures in these materials.*

*Science 31 January 2014: 519-522*

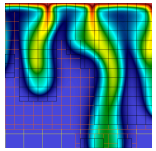
# About the Title Slide Images



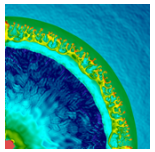
Evolution of electrical current density, parallel to magnetic field, in the Pegasus Toroidal Experiment; provided by John O'Bryan and Carl Sovinec, University of Wisconsin-Madison; Sponsored by Office of Fusion Energy Sciences



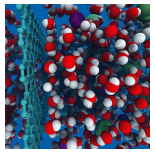
A single month from a simulation of the 20th century by the CCSM capturing wind directions, ocean surface temperatures, and sea ice concentrations. Image courtesy Gary Strand (NCAR) and copyright University Corporation for Atmospheric Research. Sponsored by Office of Biological and Environmental Research



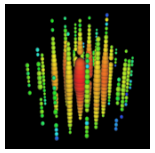
Simulation of density-driven flow for $CO_2$ storage in saline aquifers. Shown is a snapshot of the $CO_2$ concentration after onset of convection overlayed on the AMR grid. Image courtesy of George Pau and John Bell (LBNL). Sponsored by Office of Advanced Scientific Computing Research.



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


# National Energy Research Scientific Computing Center