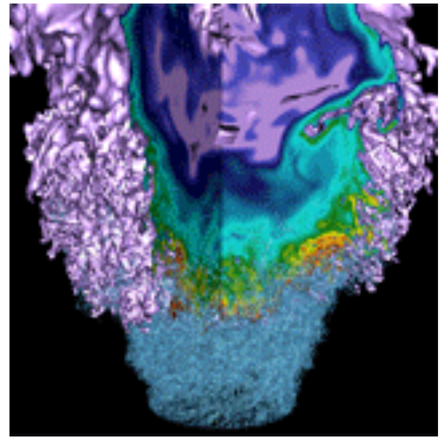
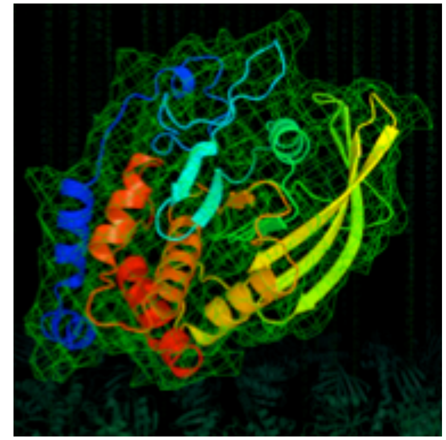
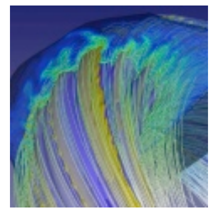
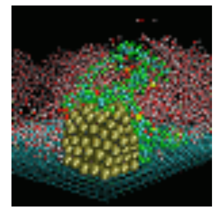
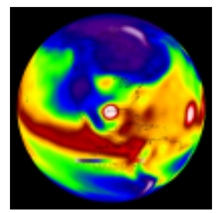
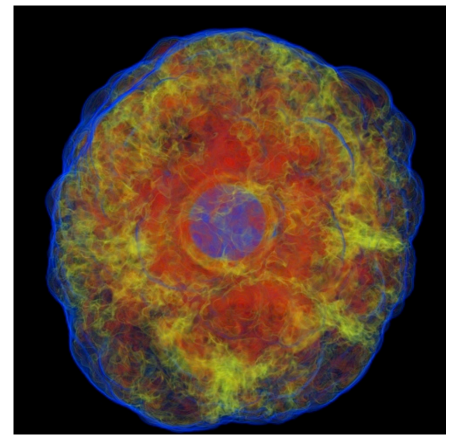
NERSC Science Highlights



NERSC

Selected User Accomplishments

March 2013

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

NERSC User Science Highlights

Materials

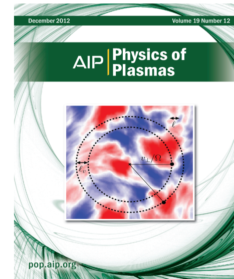
Semiconductor exciton binding energy variation explained

(Z. Wu, Colo. Sch. Mines)

Fusion

Direct simulation of freely decaying turbulence in 2-D electrostatic gyrokinetics

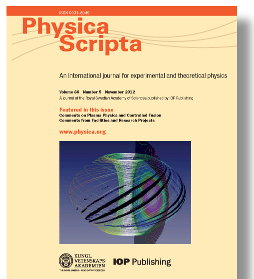
(W. Dorland, U. Maryland)

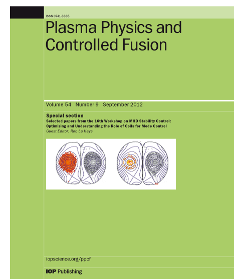


Fusion

Simulations show for the first time intrinsic stochasticity in magnetically confined toroidal plasma edges

(L. Sugiyama, MIT)





Fusion

NIMROD simulations explain DIII-D shot variability

(V. Izzo, General Atomics)

Chemistry

Study points the way toward more efficient catalysts

(S. Chen, PNNL)

Materials

High-temp superconductivity findings net researchers the first NERSC Award for High Impact Scientific Achievement

(T. Das, LANL)

U.S. DEPARTMENT OF ENERGY | Office of Science

January 2013

BERKELEY LAB

Origin of the Variation of Exciton Binding Energy in Semiconductors

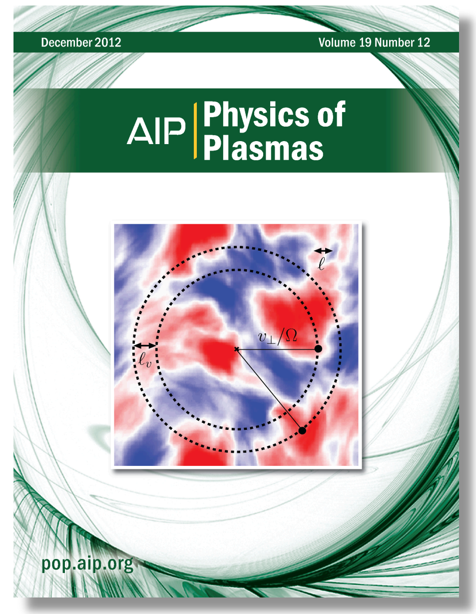
- **Exciton effects are essential to modern electronics such as photovoltaic cells, LEDs, & lasers**
  - An exciton is the electron/electron hole quasiparticle produced when light is absorbed by a seminconductor
- **But the large variation (~1 meV – 100 meV) in exciton binding energy among common semiconductors has never been fully understood.**
- **First-principles density functional theory calculations clearly show that the variation is due to localization of the exciton, which in turn is determined by the strength of semiconductor electron screening.**
- **Paves the way for understanding and predicting excitonic effects in more complicated semiconductors without resorting to much more computationally demanding techniques.**

On the Cover: Isosurfaces of valence charge density (upper panels) and exciton distribution chosen for the first issue of PRL for 2013

Physical Review Letters 110, 016402 (2013)

Freely Decaying Turbulence in 2-D Electrostatic Gyrokinetics

- **Accomplishment: Direct numerical simulation of key inherently non-linear plasma turbulence effects**
- **Motivation: Plasma turbulence plays an important role in fusion devices and various space and astrophysical situations**
  - an essential phenomenon underlying transport and particle heating
- **2nd-most read POP article in January 2013**

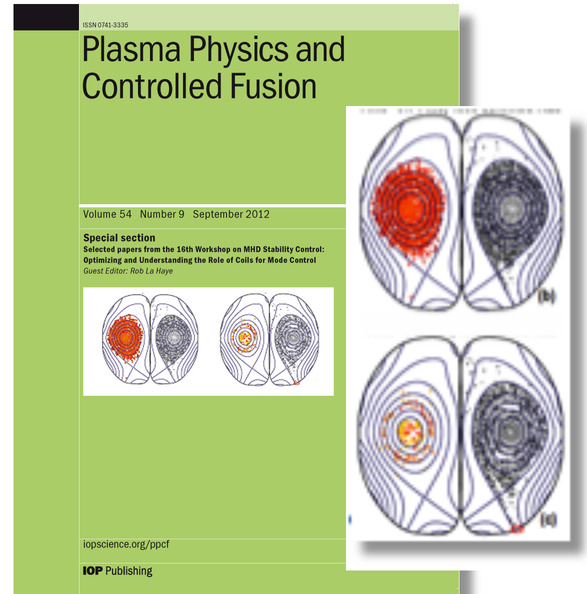


On the Cover: Colors indicating electrostatic field strength from first-of-a-kind numerical investigations of entropy cascade in phase space plasma turbulence

Physics of Plasmas 19, 122305 (2012)
PRL 103, 015033 (2009)

Predictions are Important Step Towards ITER Disruption Mitigation

- **Study of runaway electron (RE) currents that sometimes appear with tokamak plasma disruption**
  - Could be highly destructive in ITER; remains a critical unsolved issue
- **NIMROD code simulations analysed a set of six DIII-D fusion device discharges; explained shot-to-shot variations**
  - Predicts better RE confinement for shots in which higher currents were observed in DIII-D
- **Supports the hypothesis that RE deconfinement by MHD fluctuations is a major factor**
- **Validates NIMROD RE model**



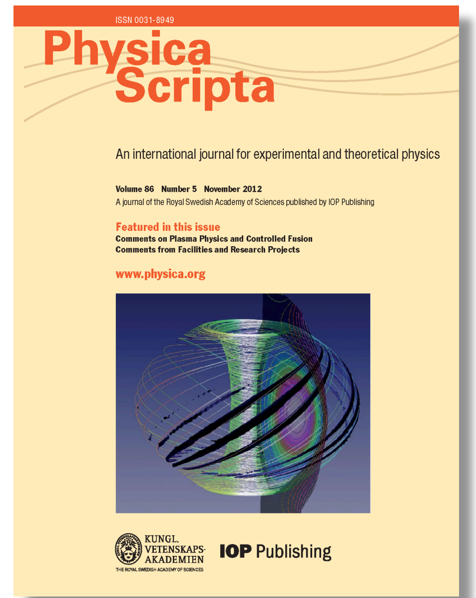
On the Cover: This issue, with selected papers from the 16th Workshop on MHD Stability Control, featured magnetic field line puncture plots and flux contours created through simulations at NERSC.

Plasma Phys. Control. Fusion 54 (2012) 095002

Intrinsic Stochasticity in Fusion Plasmas

NERSC

- **Large scale MHD numerical simulations have shown for the first time that magnetic stochasticity can be intrinsically generated in the edge of a confined toroidal plasma.**
- **Stochasticity may influence the degree of plasma confinement.**
- **Edge instabilities have the potential to be dangerously large and their control is critical for successful burning plasmas.**
- **improvement in numerical simulation techniques and computational power are starting to allow serious dynamical studies of the plasma edge.**



On the Cover: This special issue with Comments on Plasma Physics and Controlled Fusion featured the results of simulations of plasma instabilities known as Edge Localized Modes (ELMs) carried out at NERSC.

Phys. Scr. 86 (2012) 058205

Determining the Sign of the Pairing State in High-*Tc* Superconductors

- **Large-scale computation at NERSC allowed researchers to develop a theory of, and propose measurements for, certain fundamental properties of novel high-temperature superconducting materials.**

- **First NERSC Award for High Impact Scientific Achievement – Early Career – for this work and other groundbreaking contributions in superconductivity by LANL postdoc Tanmoy Das**

On the Cover: comparing computed (top) and experimental (bottom) spectra allowed testing of an important part of the gap theory in superconducting materials

J. Physics Condensed Matter
24 (18) 182201 (2012)

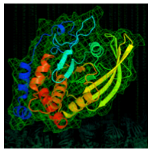
Study Points to More Efficient Catalysts

- **Simulations at NERSC and at other DOE computing centers helped explain the activity and molecular basis for an important catalyst**
  - To efficiently convert electrical energy into chemical bonds, a new generation of inexpensive, yet efficient electrocatalysts is necessary.
  - This catalyst used here is an excellent prospect: exceedingly effective for both hydrogen oxidation and production
- **Finding: Proton delivery and removal determines if the catalyst takes its highly productive form or twists into a less useful structure**
- **Conclusions from the study are thought to be broadly important, relating to the role that H_2 splitting plays in many catalytic processes.**

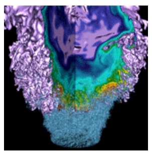
On the Cover: journal editors note that the "…accurate and comprehensive theoretical study will allow deeper understanding to guide design of more efficient catalysts for interconversion of electrical energy and fuels."

Chem. Eur. J 18 (21) 6493 (2012)

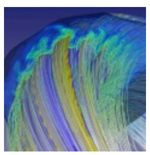
About the Title Slide Images



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)

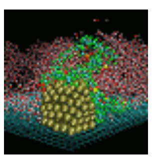


Detailed structure of a flame from a Low swirl burner combustion simulation. Image courtesy of John Bell, LBNL.

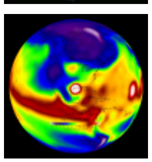


Representation of a plasma from a magnetic fusion energy simulation. Magnetic fields within the plasma are represented as white lines and the temperature is shown as blue/yellow surface (Linda Sugiyama, MIT)

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)

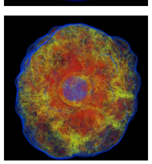


Image depicting a central engine model used in simulation of core-collapse supernovae and long gamma-ray bursts, from Christian Ott (Caltech)

National Energy Research Scientific Computing Center