

LA-UR-

12-00346

Approved for public release;  
distribution is unlimited.

*Title:*

Los Alamos National Laboratory Science & Technology  
Update  
January 30, 2012

*Author(s):*

Alison Grieggs, PADSTE  
Alan Bishop, PADSTE

*Intended for:*

LANS/LLNS Science & Technology Committee Meeting  
Livermore, CA  
January 30, 2012



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Los Alamos National Laboratory  
Science & Technology Update

By  
Alan Bishop  
Alison Grieggs

Presented to  
LANS/LLNS Science and Technology Committee Meeting  
January 30, 2012

Abstract

Dr Alan Bishop briefs the LANS/LLNS Science and Technology Committee on accomplishments, awards, FY12 priorities, and new initiatives at the committee's quarterly briefing. Topics include

- Los Alamos National Security was awarded an additional contract award term year for LANL during its 2011 performance evaluation
- FY12 and FY13 budget concerns led to creation of the LISC
- LANL staff have received prestigious external awards
- LANL named five scientists to Lab Fellows
- We have achieved many scientific accomplishments in the first quarter of FY12
- LANL has established five top science priorities for this fiscal year



# Los Alamos National Laboratory Science & Technology Update

Alan Bishop  
Acting Principal Associate Director  
Science, Technology & Engineering

January 30, 2012

# Laboratory and Washington updates

S&T Snapshot



## **LANL 2011 Performance Evaluation**

- Additional Award Term Year, LANL received 89% fee
- STE contributed to major elements
- 97% score for STE

## **Congressional Support for DOE “Exascale Plan”**

## **Strategic Tech Transfer CRADAs Support OSTP Initiatives**

## **NNSA Facility Call**

## **FY12 and FY13 Budgets**

- Generational stress for societal-Government compacts!
- Administration, Congress, OMB: renormalizing budgets to FY09 levels
- LANL focus on cost-containment and preserving key assets for future: Adapting LANL “ecosystem” for ST&E to meet this century’s national imperatives



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

UNCLASSIFIED

LA-UR-12-00XXX: 2





# FY12 Hiring Strategy: Recruit and Retain

*The Laboratory Integrated Stewardship Council (LISC) process has "introduced viscosity" in hiring and procurements.*

- *Postdoc hires and student programs continue, exempted from LISC review. To date in FY12, 15 Postdoc conversions to Scientist-2 (12 are Term appointments).*
- *Organizations are prioritizing hiring plans to align with capability areas.*
- *External Scientist hires in FY12:*
  - One Scientist-2*
  - Three Scientist-3*
  - One Scientist-5*

LANL's newest Scientist-5 external hire: **David Wolpert**

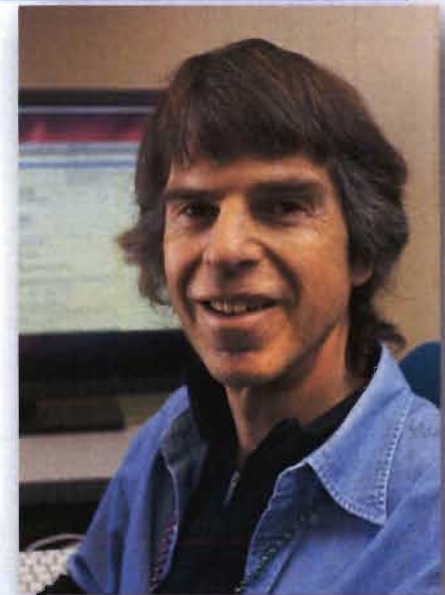
## **Recent Experience**

- Formed the Collective Intelligence group at NASA Ames Research Center
- Consulting professor in Stanford's Aeronautics and Aerospace Department
- External faculty at the Santa Fe Institute
- Ulam Scholar at the Center for Nonlinear Studies in Los Alamos (2011)

## **Research Interests**

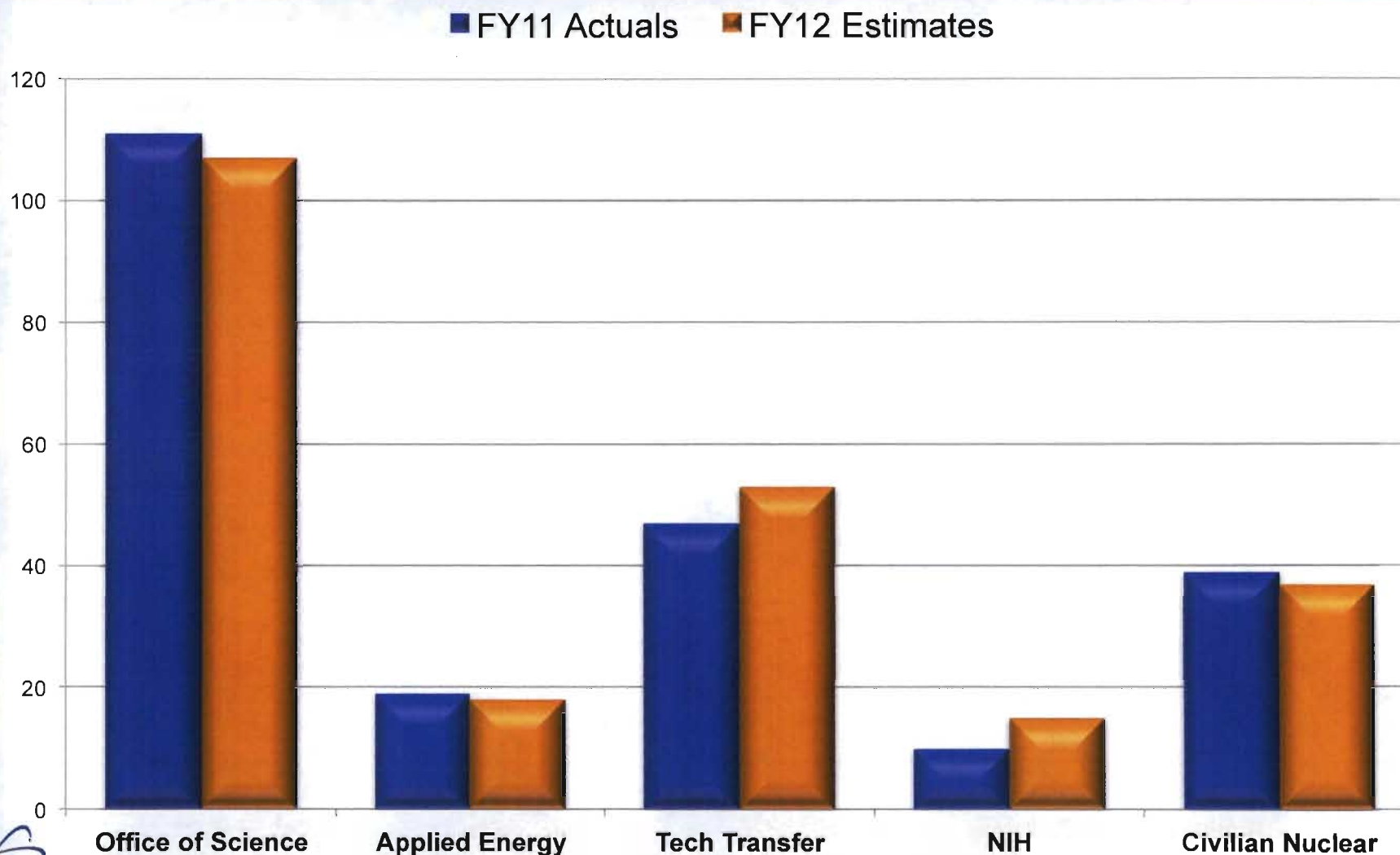
Game theory (experimental and theoretical), optimization, and Monte Carlo methods, with focus on using machine learning technology to improve those disciplines. Also works in information theory, complexity, and the foundations of physics and inference.

Authored two books, three patents, ~100 refereed papers, numerous awards.

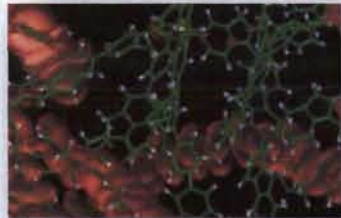


LA-UR-12-00XXX: 3

# Science & Energy Programs Funding: Comparing FY11 actuals vs FY12 estimates



# New LDRD DR Projects for FY12: Strategically aligned



*Organic Electronic Materials*



*TeV jets*



*Predicting Climate  
Impacts in the Arctic*

- Computational Co-Design
- Organic Electronic Materials: Designing and Creating Functional Interfaces
- Energy Storage
- Dynamic Earthquake Triggering, Granular Physics and Earthquake Forecasting
- Genetically Encoded Materials: Libraries of Stimuli-responsive Polymers
- TeV Jets: Nature's Particle Accelerators
- Integrated Modeling of Perturbations in Atmospheres for Conjunction Tracking
- Hydrodynamical Mix Studies at the National Ignition Facility (U)
- Advancing the Fundamental Understanding of Fission (U)
- Predicting Climate Impacts and Feedbacks in the Terrestrial Arctic
- Physics Beyond the Standard Model with the Long-Baseline Neutrino Expt.
- Hierarchical Sparse Models for Robust Analysis of Video Data
- Elucidating Humankind's Evolving Environment
- Plutonium-242: A National Resource for the Fundamental Understanding of 5f Electrons
- Modern Challenges in Actinide Science
- Quantum Science: From Information to Materials



# Our scientists continue to receive prestigious individual external awards

Achievements: Awards



**Mark Chadwick**  
E.O. Lawrence Award



**David Chavez**  
E.O. Lawrence Award



**Christine Anderson-Cook**  
American Society for  
Quality Fellow



**Miles Baron**  
National Intelligence  
Medallion



**Nancy Jo Nicholas**  
Institute of Nuclear  
Materials Mgmt. Fellow



**Frank Pabian**  
Visiting Fellow, Stanford  
Center for International  
Security and Cooperation



**Dane Spearing**  
American Ceramic  
Society Fellow



We've had a banner year with American Association for the Advancement of Science fellowships...

Achievements: Awards



**Alexander Balatsky**



**Byron Goldstein**



**John Gordon**



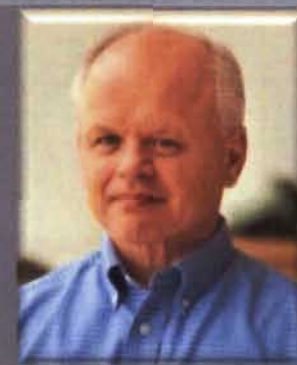
**Quanxia Jia**



**Jacqueline Kiplinger**



**Jeanne Robinson**



**Richard Sayre**

## ...and American Physical Society Fellows

Achievements: Awards



**Michael Chertkov**



**Timothy Germann**



**Fernando Grinstein**



**Marcelo Jaime**



**Bogdan Mihaila**



**Dean Preston**



**Charles Reichhardt**



**Cynthia Reichhardt**



# LANL recognizes the scientific excellence of Laboratory Fellows

Achievements: Awards



**Bruce Carlsten**



**Michael Leitch**



**Michael MacInnes**



**Richard Martin**



**Amit Misra**

*The Fellows we welcome this year represent the deeply talented pool of scientists at Los Alamos—world leaders in their fields—and we are honored that they are part of our national security science team. Los Alamos has a history of vital contributions, both in basic science and in applied science advancing national security, and these individuals are essential to maintaining that capability."*

*Alan Bishop, PADSTE*



# Cybersecurity: National Cybersecurity Innovation Award

Achievements: Awards



LANL partnered with industry to build unique capabilities that leverage **VMware's** security products.

- Created "*Infrastructure on Demand*" platform—a dynamic cloud portal—that features an inventive cloud security and automation architecture to reduce a 30-day server-provisioning process to 30 minutes.
- Users can leverage this portal to automatically request and provision virtual systems to meet their unique needs.

This work was supported by LANL's IS&T capabilities.

*Innovation provides cybersecurity and manages virtual computers deployed in the cloud environment*



*InformationWeek 500 Award*

**Los Alamos**  
NATIONAL LABORATORY  
EST. 1943

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

UNCLASSIFIED

LA-UR-12-00XXX LAQR-12-00XXX: 10



# Science that Matters Pillars: Ensuring vitality in core capabilities is essential for our mission

## Materials for the Future

"Controlled functionality" across three themes: defects and interfaces, extreme environments, and emergent phenomena.



## Integrating Information, Science, and Technology for Prediction

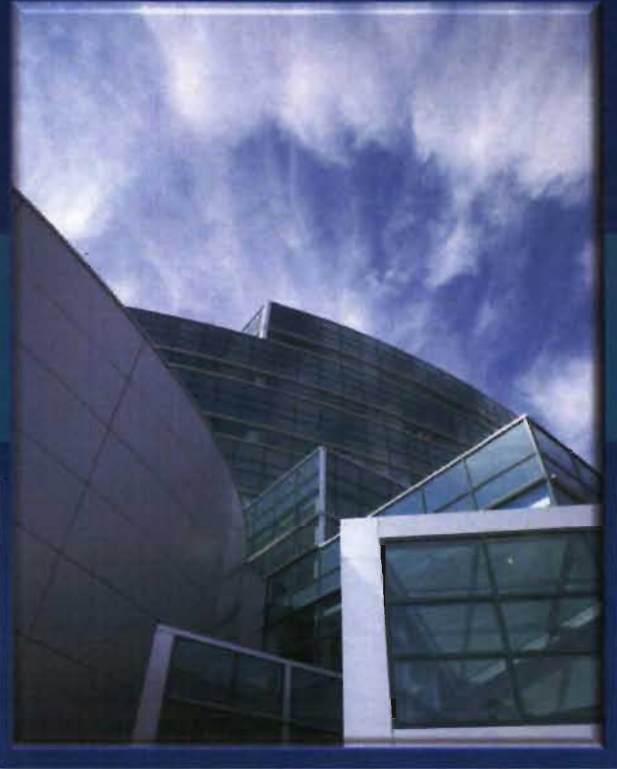
Predicting materials performance, situational awareness, and energy-climate impacts and energy infrastructure across three cross-cutting IST areas: data science at scale, computational co-design, and complex network science.

## Science of Signatures

"Meaningful measures and knowledge generation in complex environments" across three science themes: discover signatures, revolutionize measurements, and forward deployment.







## FY12/First Quarter STE Highlights



# Strategic Partnerships for Tech Maturation (FY12/Q1 Highlights)

**EMC<sup>2</sup>** Visit and signing ceremony with EMC senior management (VP, CTO) to initiate a new CRADA (*software and high performance computing*)



Visit by Boeing senior management (General Manager, VP) to initiate a new umbrella CRADA and first project (*Supercooled droplet detection*)

**P&G** Visit by P&G senior management (VP, General Manager) to enhance ongoing CRADA projects (*Nonpetroleum feedstocks, modeling and simulation*)



New license agreement with Harris Corporation to develop Quantum Encryption (*QES and QKarD*)



New CRADA with TerraPower (*Irradiation testing and microstructural analysis*)

**SHARP** New CRADA with Sharp Corporation (*Quantum dot solar cells*)



New CRADA with Chevron (*Explosive fracturing*) and new license agreement (*Swept frequency acoustic interferometry*)



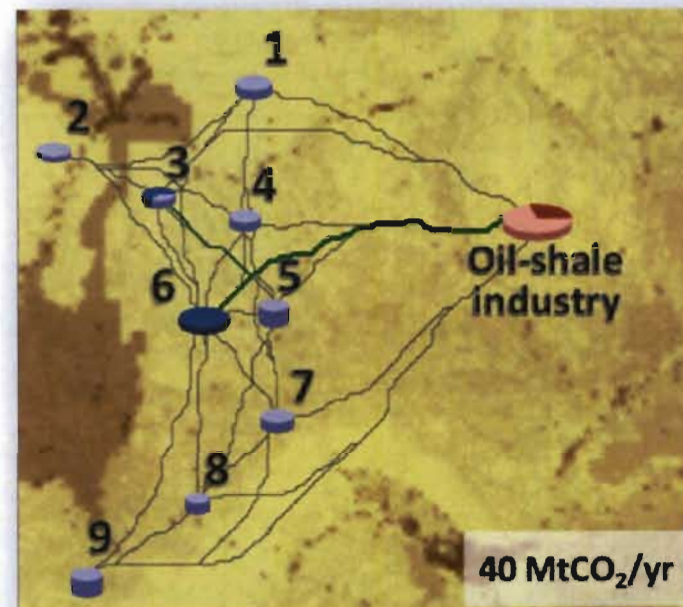
## Energy Security mission: Journal highlights CO<sub>2</sub> capture and storage

Carbon dioxide (CO<sub>2</sub>) capture and storage is a critical technology to reduce emissions of greenhouse gases.

*Environmental Science & Technology* selected a recently published paper for inclusion in a special issue of the journal "Water-Energy Nexus."

CO<sub>2</sub> sequestration site-screening approach involves identifying appropriate sequestration basin, analyzing sequestration target formations, defining surface sites, designing infrastructure, and analyzing CO<sub>2</sub> transport and storage costs.

*Provides approach to CO<sub>2</sub> sequestration site screening for industries or energy development policies*



*Spatial infrastructure deployment for capturing, transporting, and storing CO<sub>2</sub>. Blue cylinders represent sinks, and red cylinder represents CO<sub>2</sub> production. Lines show candidate pipeline routes.*

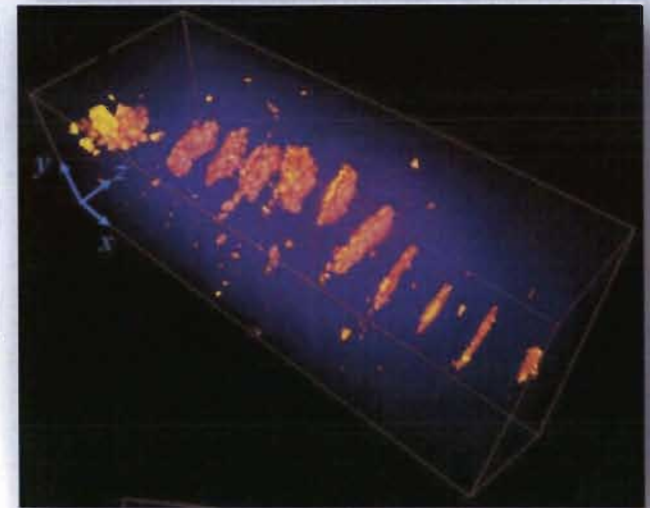


## Global Security mission:

A fast and inexpensive method to fabricate 3D metamaterials

*Fabrication method enables fast and inexpensive 3D-materials design of metamaterials (manmade structures that can manipulate electromagnetic and acoustic waves to create invisibility cloaks, subwavelength focusing, and shielding). The combination of their intriguing properties positions metamaterials for a significant technological impact.*

- Bench-top process fabricates 3D periodic structure using high-frequency acoustic waves in a resonator cavity. (*Review of Scientific Instruments*, 2011)
- Acoustic waves direct nanoparticles toward the nodes of the standing wave field to form parallel periodic planes within a 3D epoxy matrix.
- Creates materials with a periodicity of the pattern in the range of 1-100 micron: a gap in existing fabrication technology.



*Nanocomposite metamaterial containing diamond nanoparticles*



## Energy Security mission: Technical leadership in algal biofuel research

- José Olivares and Richard Sayre established the *Algal Research* journal and organized the 1<sup>st</sup> and 2<sup>nd</sup> International Conference on Algal Biomass, Biofuels, and Bioproducts.
- *Biofuels Digest* named Olivares to “Top 100 People in Bioenergy.”
- NAABB chose LANL’s R&D100 Award-winning Ultrasonic Algal Biofuel Harvester process for Phase II development.

### Research updates

- Discovered potential key to degrade cellulosic biomass. (*Journal of the American Chemical Society*, 2011)
- Developed mild conditions to open the furan rings formed during the breakdown of lignocellulose. (*Green Chemistry*, 2011)
- Flow cytometry cell-sorting selected high-lipid-producing cells from cultures under low nutrient conditions (nitrate deprivation) to produce 20-30% more lipids.



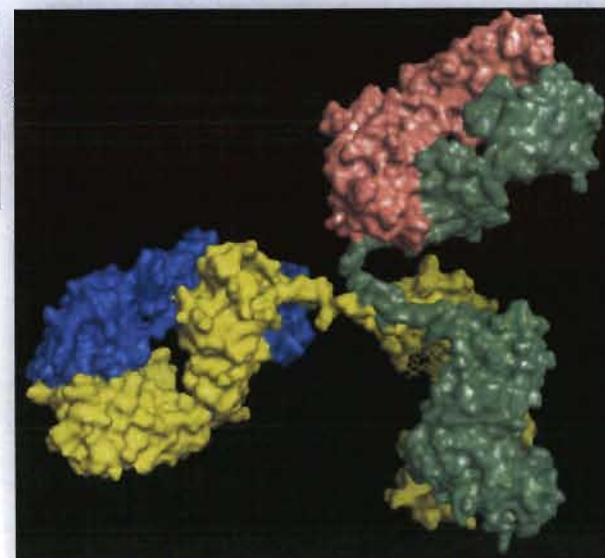
*Integration of theory, simulation, and experiment enables scientific innovation*

## Global Security mission: Antibody library project could unlock mysteries

*Broad availability of antibodies against all human proteins could facilitate the understanding of human disease and provide targets for therapeutic intervention.*

**Andrew Bradbury leads a new NIH consortium grant to develop a pilot high-throughput antibody selection pipeline**—which could unlock mysteries of human genome function.

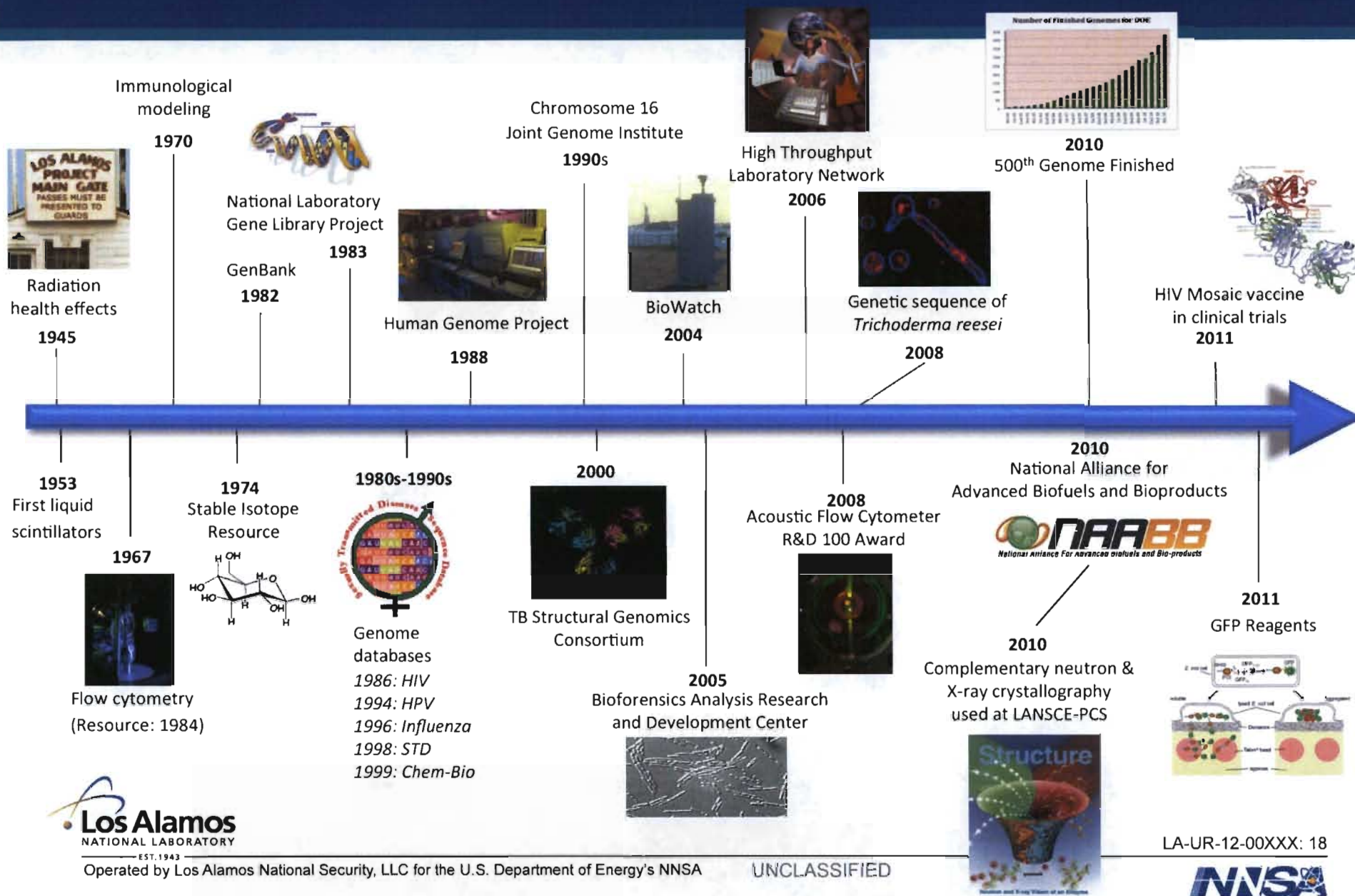
- Expected to increase through-put by 100-fold and dramatically decrease cost.
- Will use bacteria and bakers yeast to generate antibody libraries, thus avoiding the use of animals to generate antibodies.
- Will enable assessment of gene function through binding of antibodies to the products of the genes.
- Builds on the Human Genome project and leverages technology developed at LANL (flow cytometry, antibody libraries, fluorescent proteins).



*Structure of an antibody*



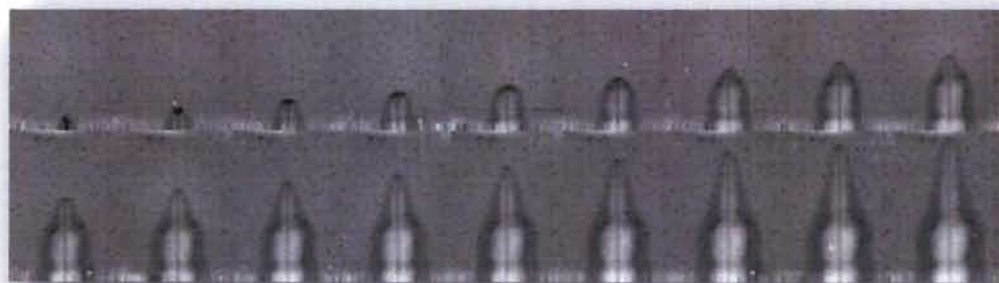
# LANL has a rich history of contributions to Bioscience R&D



# Nuclear Deterrence and Global Security missions: Proton radiography examines granular flow

- Granular materials are vital to industries ranging from mining to ballistic mitigation.
- Macroscopic solid grains under dynamic load have different physical properties from either a bulk solid or a liquid.
- Lack of diagnostic techniques at such high pressures and velocities has limited shock compression studies.
- Proton radiography measured the velocity field of sand.

*The 2D mesoscale modeling under development will include asymmetric loading and grain level effects for prediction of the penetration depth and overall effectiveness of the projectile*

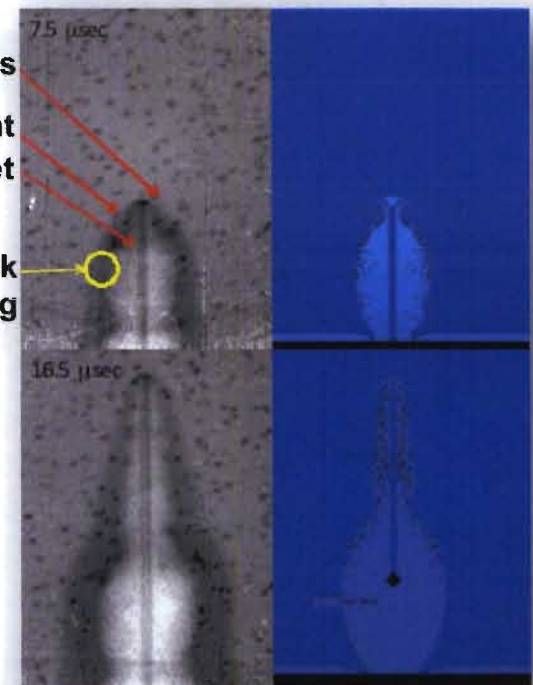


*A copper "viper" jet penetrating a target of dry sand, beginning at 1.5 microsecond after impact. Images are separated by 1 microsecond.*

W tracer particles

Shock front  
Viper jet

3D shock  
broadening



*Comparison of experimental data (left) with simulation (right).*

LA-UR-12-00XXX: 19



# Global Security mission: Mars rover launches with two LANL instruments and fuel



*NASA artist's conception of the rover using the ChemCam instrument*



*Scientists prepare to test the laser for ChemCam in the LANL cleanroom*

*LANL has a long history of developing sensors and analytical instruments for space applications*

**Mars Science Laboratory rover *Curiosity* is the largest mission ever attempted to another planet. The mission's goal is to determine if environmental conditions favorable to microbial life ever existed at the site.**

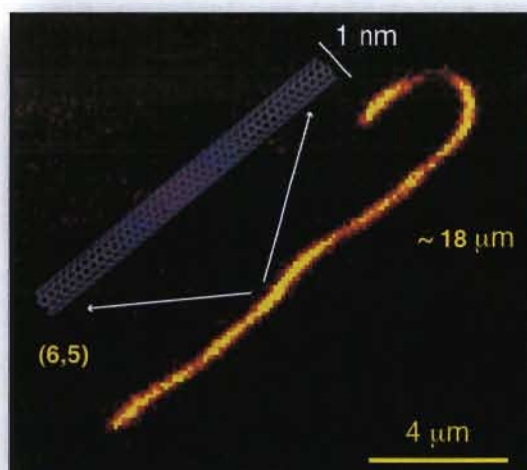
**LANL is the largest contributor after NASA.**

- Developed 2 of 10 analytical instruments.
- Led development of the ChemCam instrument, including a Laser-Induced Breakdown Spectrometer (LIBS) to determine the elemental composition of samples up to 7 meters away.
- Co-led development of the CheMin instrument to provide mineralogical analyses.
- Provided the plutonium-238 fueled clads for the heat-producing Multi-Mission Radioisotope Thermoelectric Generator unit.

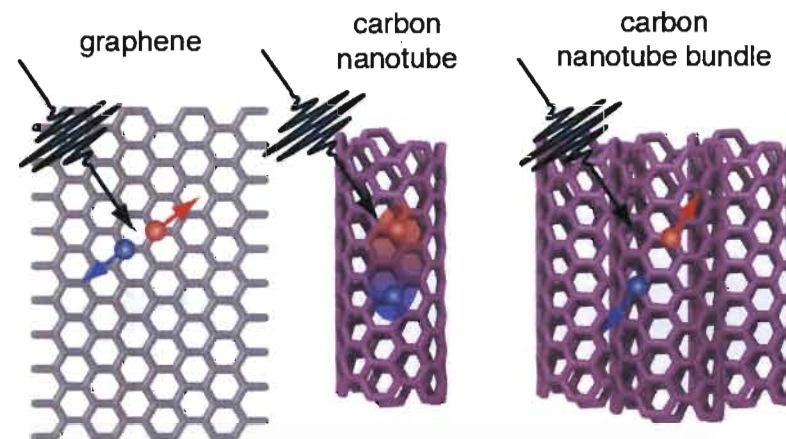
# Global Security and Energy Security missions: Single-wall carbon nanotubes show promise

*Provides an understanding of how the local chemical environment can introduce perturbations in the underlying nanotube electronic structure that alter light-emission and transport characteristics*

LANL imaged exciton quenching in nanotubes during the early stages of chemical doping. (*Nature Nanotechnology*, 2012). The nanotube lattice provides a 1D channel for transport of exciton quenchers.



Left: artist's illustration of the nanotube's structure; right: photoluminescence microscopy image of a carbon nanotube



Schematic of light absorption and charge separation of graphene, carbon nanotubes, carbon nanotube bundles

Researchers showed how electronic dimensionality can be altered in a nanotube aggregate through charge transfer excitons. (*Physical Review Letters*, 2011)



## Global Security mission:

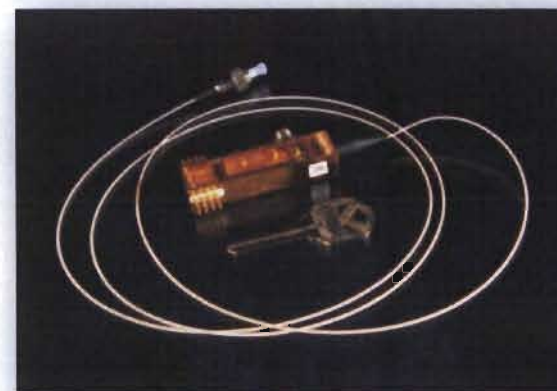
QKarD brings quantum cryptography to handheld devices

*QKarD patent-pending technology is licensable for security systems in banking, online transactions, access to secure facilities, border crossings, digital rights management controls, and electronic voting.*

**LANL developed an impenetrable line of defense known as QKarD (Quantum Smart Card).**

QKarD has many advantages over current key distribution methods:

- Uses polarized single photons to generate and distribute secret keys with much higher security and much lower computational requirements.
- Laws of quantum physics and information theory ensure that these keys can never be cracked.
- QKarD fits into smaller devices, such as a smartphone, wireless credit card, or identification card for mobile applications.



*QKarD uses miniaturized quantum cryptography technology. The transmitter communicates with a designated central trusted authority to generate random cryptographic keys to encode and decode information.*

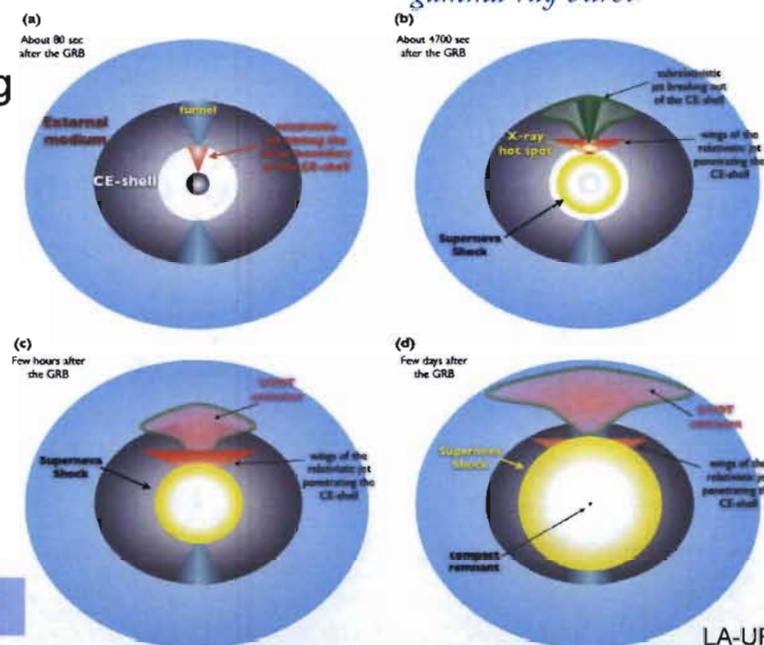
# Global Security and Nuclear Deterrence missions: Modeling and simulation explain unusual gamma-ray burst

A multi-national team analyzed a powerful, long-lasting gamma-ray burst that occurred on Christmas Day 2010 and characterized it as a neutron star spiraling into the heart of a companion star. (*Nature*, 2011)

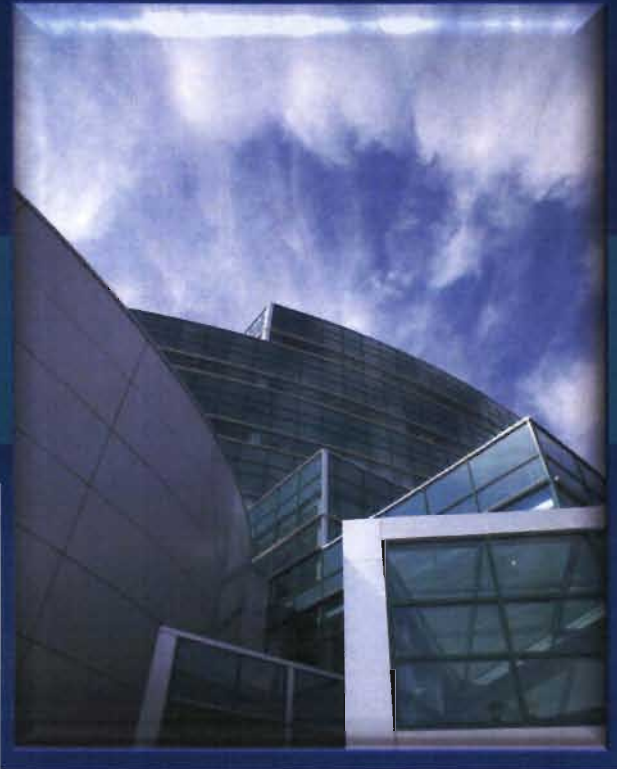
- Chris Fryer realized that the peculiar evolution of the thermal emission could be explained by the Helium Merger Model [Fryer and Woosley (UCSD), 1998].
- Chris Fryer and Wesley Even are using DOE's ASC codes (RAGE on LANL's Yellowrail computer) to examine the emission of the burst in more detail.



Artist's conception of the neutron star/helium star collision and resulting gamma-ray burst.



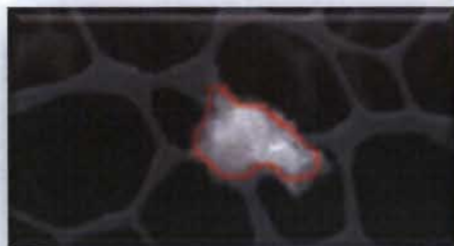




# FY12 STE Priority Updates

# LANL Science Priorities for FY12

**Capability-based recruitment and retention for excellence and impact**



**Science of Signatures:**  
Nuclear Forensics and LANS Contract Award Term Measure

**Exascale Computing:**  
LANL-led Exascale Co-design Center for Materials in Extreme Environments



**MaRIE:**  
Respond to the NNSA DP Science Facility Call

**Plutonium Science:**  
Implement Science Strategy and key facilities





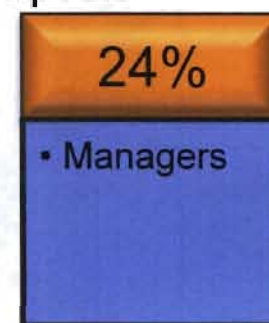
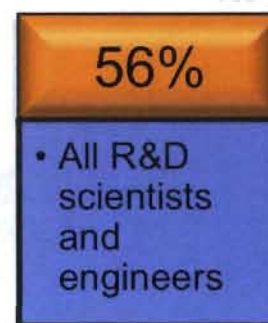
# Capability-based recruitment and retention: Return on “Student and Postdoc Pipeline” Investments

**Student interns and postdocs contribute significantly to LANL’s programmatic work, publications, citations, conference presentations, inventions, tech transfer, science education outreach, collaborative R&D and LANL’s international reputation.**

Percentage of **new hires** in FY11  
who were former students or postdocs



Percentage of the **total LANL population**  
who were former students or postdocs



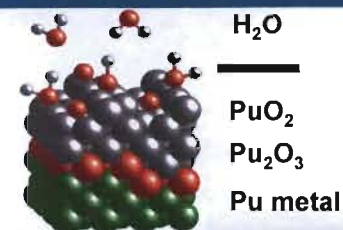
*Critical to LANL’s STE ecosystem and the country’s STE competitiveness!*

# Science of Signatures: FY12 Award Term



**Capability reviews identified a lack of “basic science” in the nuclear sensing area. The FY12 LANS Contract Award Term Measure includes four remedies:**

- **Develop Science of Signatures strategic plan with an implementation plan for nuclear detection.**
- **Develop prioritized equipment list for laboratory space in RLUOB, in conjunction with Plutonium Strategy.**
- **Focus institutional investments in nuclear science and signature-detection and -measurement capabilities:**
  - Update LDRD Grand Challenges targets
  - Equipment investment opportunities
  - Collaborate with LANL Institutes and Centers
  - Infrastructure and facilities planning
- **Install and operate Secondary Ion Mass Spectrometer and 700-MHz nuclear magnetic resonance instrument.**





# Los Alamos National Laboratory and the Next Decade of Supercomputing

## Mission Critical

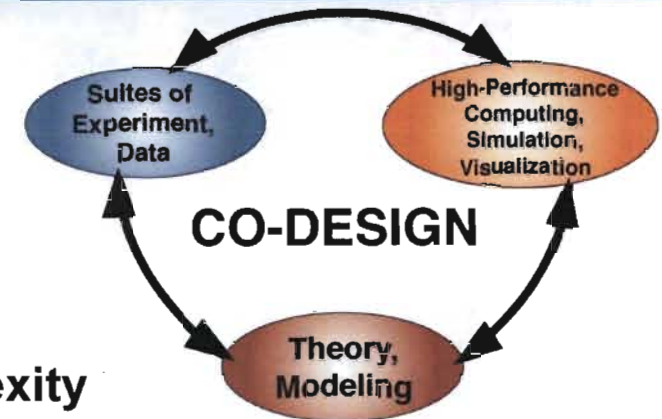
- Nuclear Weapons Stewardship
- NN, Energy, Climate, Environment, Situational Awareness, Cyber, ....
- Technology Transfer and Economic Competitiveness

## Simulation Science and the Century of Complexity

- Advanced computing now a mature element in the “Scientific Method” for Complex Systems
  - ◆ Multiscale, Multiphysics, Extremal Events, UQ, ...
  - ◆ Component and Integral (System) Codes
  - ◆ Compute- and Data-Intensive Computing

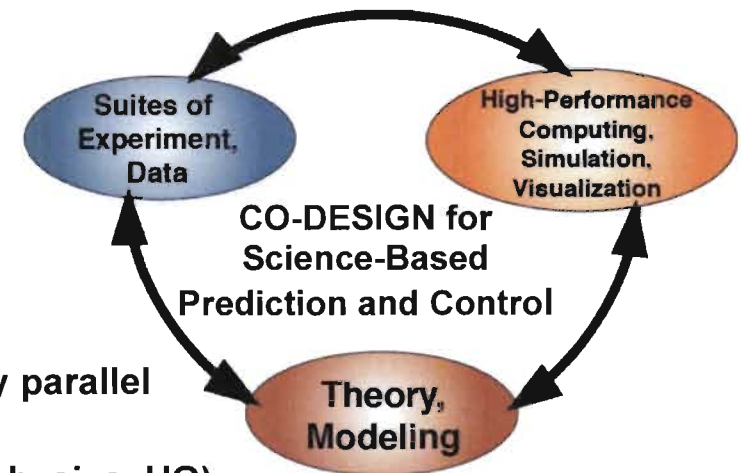
## LANL must maximize mission and discipline impact

- Coordination across PADWP, PADGS, and PADSTE
- Computational Science is an integrating discipline; must work hand-in-hand with experiments and observations across natural and social sciences and engineering
- Co-Design Teams



# High-Performance Computing at a critical time of challenges and opportunities

- High expectations (from White House, DOE, industry...) as fundamental enabling capability: Accelerating the discovery and prediction to impact and commercialization cycles to meet (inter-)national imperatives!
- Major (disruptive) technology transitions
  - Hybrid/multicore... parallelism not clock speed
  - Cooling, power, resiliency, concurrency, file systems, networking, agile programming environments for broad S,T&E portfolio  
... **managing the complexity trade-offs**
- Massive platforms AND “Cloud” distributed, massively parallel
- Full Systems (“Engineering Metrics,” Multiscale/Multiphysics, UQ)
- Compute-and-store AND data-intensive frontiers: data curation, access, security
  - Real-Time, Predictive Analytics
- Training the next generation of leaders



*The DOE road to “Exascale”:*

*Multi-Lab associations, including vendor partners*

*Co-Design Centers (**Applications, Algorithms, Architectures**)*



# US Exascale Computing Leadership

**DOE's Exascale Initiative: Exascale (and beyond) will have many applications but needs a commercially viable path**

## Mostly familiar issues

- Role of industry-government relations
- Role of industry-laboratory relations
- External threats (Japan, Europe...China)
- R&D vs Platform timetable: The "NIF" dilemma

## But new context for LANL

- DOE (NNSA & SC) integrated plan
- HPC's new maturity as a tool for S,T&E
- Role of (and business advantage of) LANL to integrate assets and avoid silos (at Labs and DOE)
  - ◆ Maximize impact for S,T&E; US economic competitiveness
  - ◆ "Co-design" (proactive integration) better than "Tech Push vs Apps Pull"



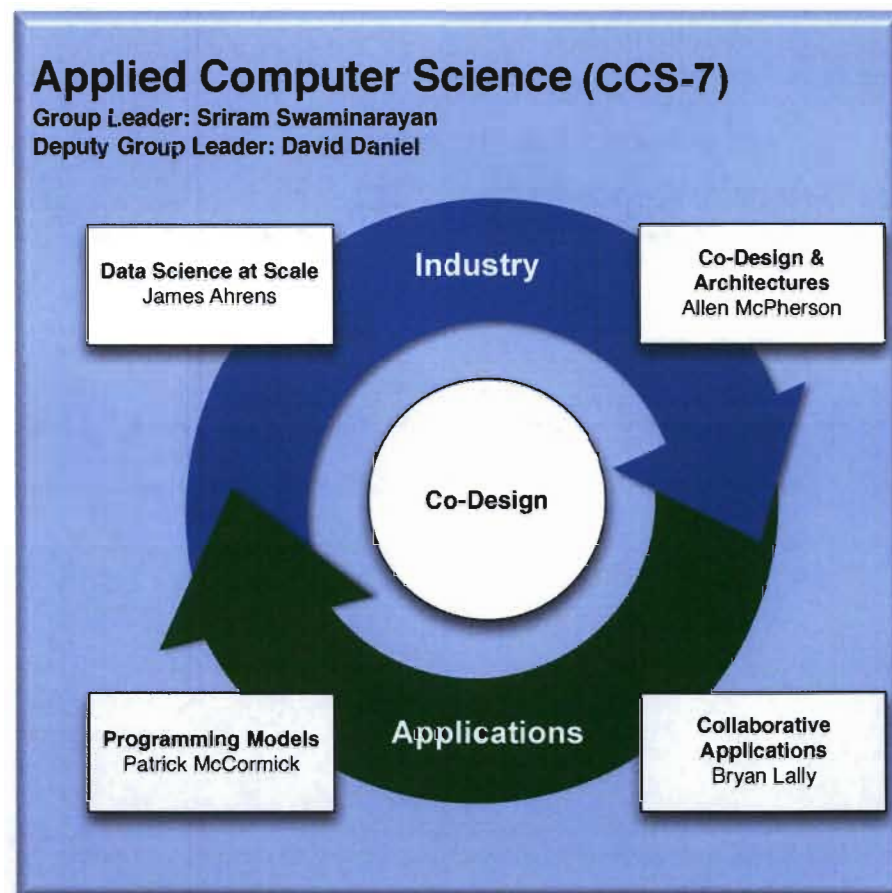
*ExMatEx is one of three DOE ASCR-funded exascale co-design centers. The center focuses on extreme-scale simulation of materials properties in extreme environments. The project emphasizes multi-scale models, computer science, and validation in one co-design process designed to move materials simulation into the exascale era.*

*Classified update on this topic scheduled for April 2012 meeting*

## “Collaborative” Design @ <http://codesign.lanl.gov/>

**Based on our GPU and Roadrunner experience—and the challenges of Exascale—LANL has refocused Computer Science activities to emphasize internal and external collaboration**

- Led to the design and formation of a new CS, co-design-focused group in late 2009
- Has become the heart of our CS co-design efforts (both externally and internally)
- We are deliberately avoiding a traditional academic separation of disciplines
  - ◆ “Fractal” nature of interactions is now on the critical path
  - ◆ Cross-discipline interactions at the micro- and macro-scale
  - ◆ Education is critical, including industry interactions





Education is a key component of our success in completing this transition to a Co-Design mindset and structure

### External Training Activities

More than 100 LANL staff from all disciplines sent to “deep dive” courses

### Internal Activities

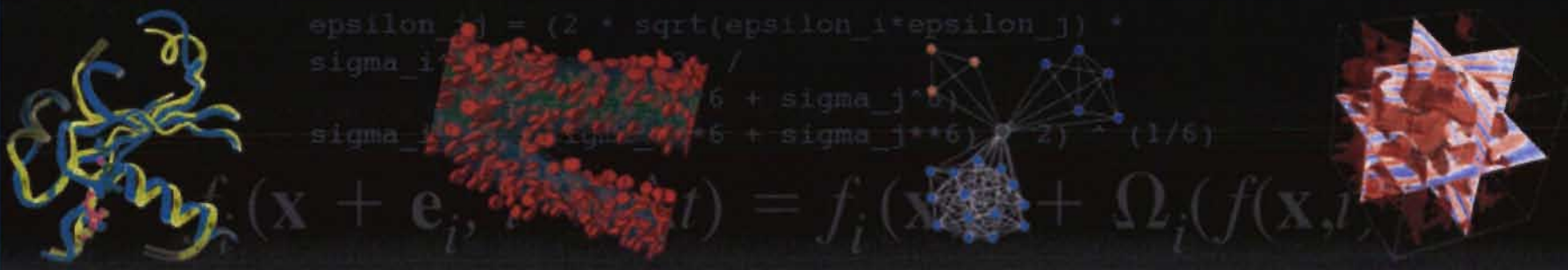
- One week every month: CS-led courses focus on critical topics (est. 2011)
- “*Hack-a-Thons*”: academic, internal, and industry hands-on over several days (Stanford, summer 2011; Intel Labs, early 2012)

### Co-Design Summer School (est. 2011)

- Cross-disciplinary graduate students and postdocs team with each other, LANL mentors, and staff to explore aspects of future generations of computing systems
- Establishing industry participation
- Establishing this interdisciplinary mindset is critical for the future



# Harvard partnership for training



*"We are bringing together a range of people who have knowledge in computation but also interest in pursuing computational approaches... That focus also extends outside the academy to include individuals from industry and national laboratories to understand computational needs in "the real world."*

*Efthimios Kaxiras, Professor of pure and applied physics at Harvard and Director of IACS*

In 2011, Harvard University established the Institute of Applied Computer Science, within its School of Engineering and Applied Sciences, to launch a unique interdisciplinary education and research program in computation science and engineering:

- Creates an intellectual home for faculty and students applying computational methods to major challenges in science
- Enhances existing courses in applied mathematics and computation, and develops new computational science courses and research opportunities

DOE supports the IACS, and the national laboratories are involved in its success and developing the new curriculum (Internships, Teaching).





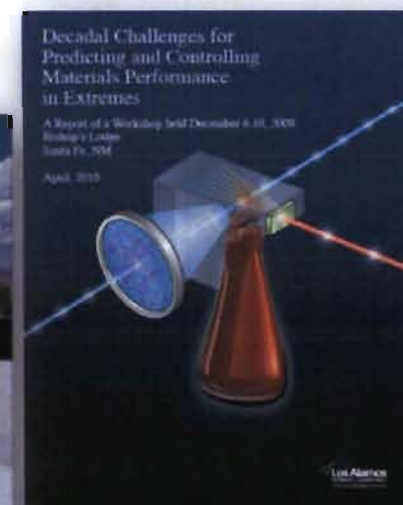
We have not yet achieved a predictive, process-aware understanding of materials performance

## Materials research is on the brink of a new era— from observation of performance to control of properties

The confluence of unprecedented experimental capabilities (e.g., 4<sup>th</sup> generation light sources, controlled synthesis and characterization, ...) and simulation advances are providing remarkable insights at length and time scales previously inaccessible

### New capabilities will be needed to realize this vision:

- *In situ*, dynamic measurements  
*simultaneous scattering & imaging*
- of well-controlled and characterized materials  
*advanced synthesis and characterization*
- in extreme environments  
*dynamic loading, irradiation*
- coupled with predictive modeling and simulation  
*materials design & discovery*



*"MaRIE 1.0," building on LANSCE success, is a key first step towards this vision*



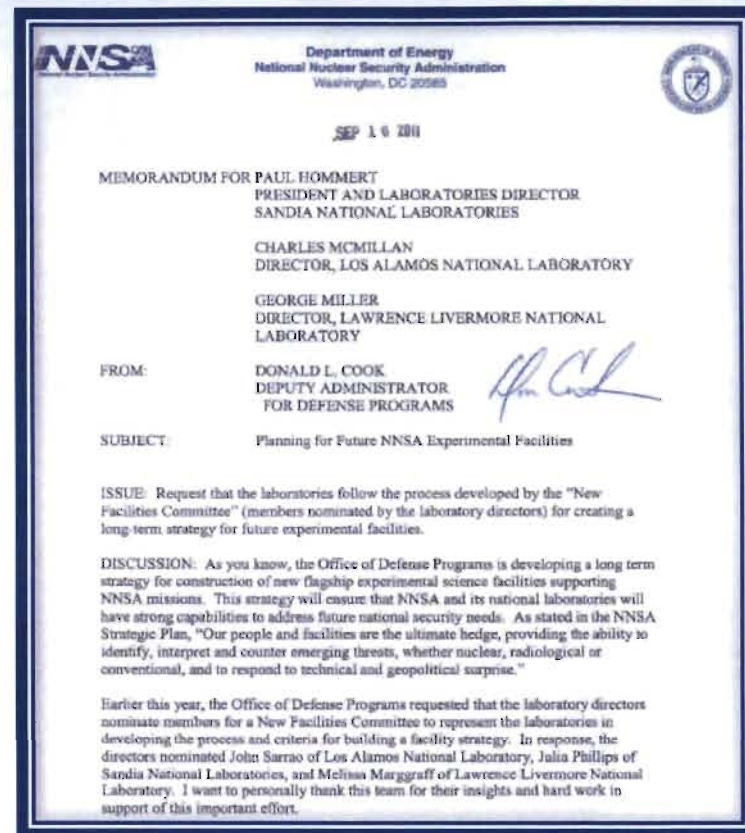
# LANL, SNL & LLNL are actively working responses to the NNSA New Facilities Call

## LANL Priorities

- MaRIE 1.0
- Nuclear Science Complex (WNR+)
- HILL (High Intensity Laser Lab)
- 3 GeV pRad

## Schedule

- |         |  |
|---------|--|
| 2/15/12 | Tri-Lab <i>Facility Roadmap</i> , up to four proposals/Lab   |
| 4/01/12 | NNSA convenes an external committee to review proposals and roadmap  |
| 7/01/12 | Second-round review  |
| 8/01/12 | NNSA integrates <i>Facility Roadmap</i> into broader planning framework; best and most urgent proposals move expeditiously to CD-0 |







# “First Experiments” demonstrate how MaRIE 1.0 meets key NNSA mission challenges

## Manage the nuclear weapons stockpile

Understand the condition of the nuclear stockpile



Extend the life of U.S. nuclear warheads

### Dynamic Materials Performance

### Process Aware Manufacturing

#### Initiation

*Multiphase High Explosive Evolution*

*High Explosive Functionality by Design*

*Dynamic Performance of Pu & Surrogate Metals and Alloys*

*Predicting Interfacial Microstructure and Strain Evolution*

*Turbulent Material Mixing in Variable Density Flows*

*Controlled Solidification and Phase Transformations*

#### Burn

## Strengthen the ST&E Base

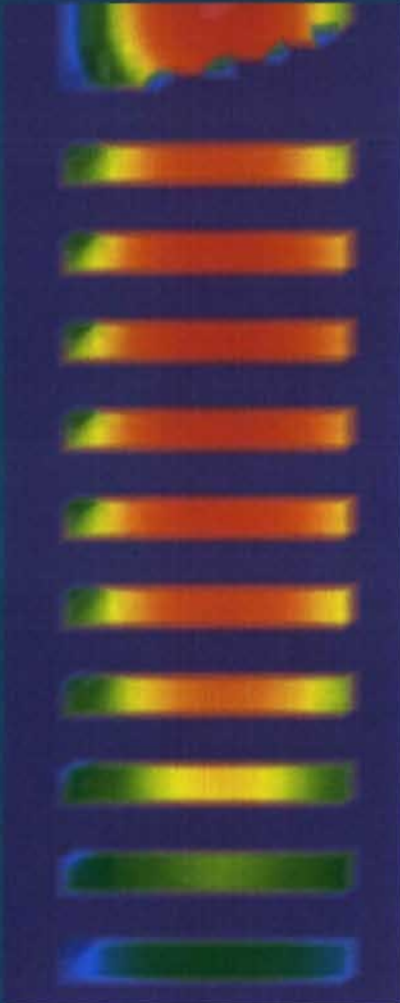
- Invest in technical workforce
- Shape the infrastructure

Protect against technological surprise

Broaden our understanding of future needs

# Plutonium Science: Implement Science Strategy and Key Facilities

FY12 Priorities: Plutonium Science



## FY12/Q1 Updates

- The *Actinides and Correlated Electron Materials* component of the *Materials Strategy Implementation Plan* was completed.
- Pu-242: Large single crystals prepared for neutron scattering at LANSCE.
- First observation of the Pu-239 nuclear magnetic resonance (NMR) transition.
- New procedure developed for shipping small R&D plutonium samples between LANL and DOE national user facilities.
- Submission of the LANL Product Based Certification white paper to NNSA Defense Programs.
- LANL programs invited to Savannah River Site for a Plutonium Solubility Expert Peer Review to evaluate radiological risk of residual plutonium (F Tank).



# The US needs LANL as a premier National Security Sciences Lab more than ever in this century!



Accelerating discovery-to-innovation for technology delivery and mission impact

Interdisciplinary science of systems at scale: From understanding to prediction



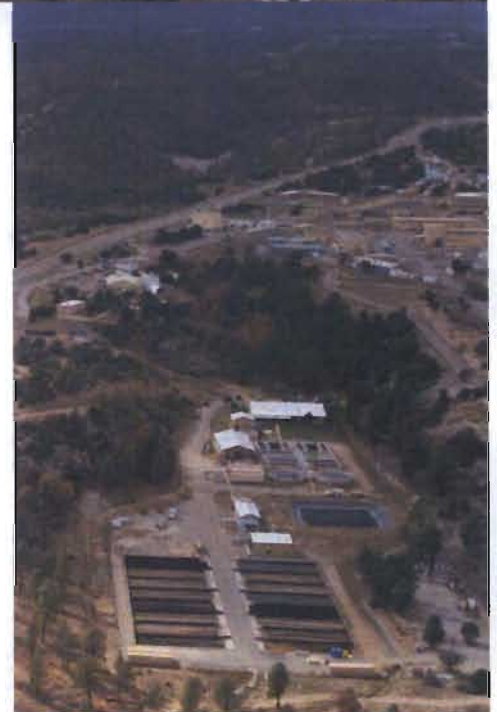
Sustaining the environment for success

- excellent people
- exciting scientific challenges
- unique facilities/infrastructure

# Facility Updates: Space improvements are scheduled in the Long-Range Development Plan



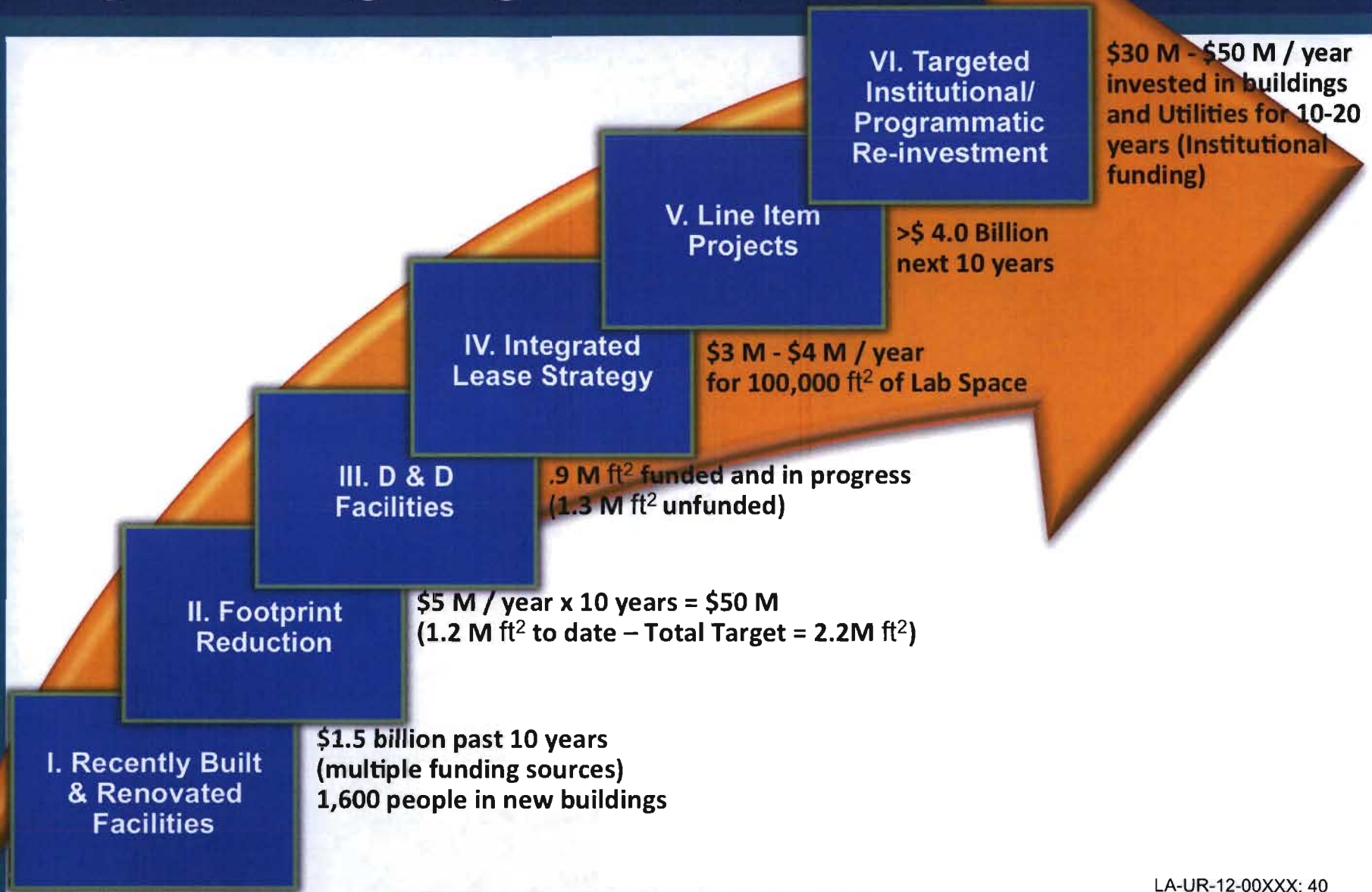
- Planned improvements will impact 72,000 ft<sup>2</sup>
  - ◆ 7,000 ft<sup>2</sup> in Research Park converted from office to laboratory space
  - ◆ 25,000 ft<sup>2</sup> of lab space refurbished (TA-59-1, MSL Build Out, Physics, TA-46, etc.)
  - ◆ 30,000 ft<sup>2</sup> of lab space improved with new mechanical system equipment
  - ◆ 10,000 ft<sup>2</sup> of new lab space in design phase (at TA-48)
- Refurbishment of an additional 50,000 ft<sup>2</sup> research/office space scheduled
- An RFI to acquire up to 100,000 ft<sup>2</sup> of new laboratory leased space was issued in January





# Integrated Long Range Development Plan

FY12 Priorities: Investments



EST. 1943

# Effective communication amplifies LANL's scientific excellence and impact

## **Craft messages in science**

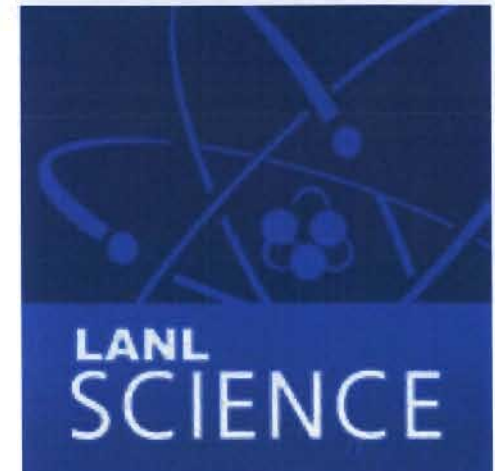
Achievements and awards, capability pillars,  
national & international impacts, programs:  
Discovery → Innovation → Impact

## **Develop integrated strategy across organizations for communicating science accomplishments**

## **Develop strategy and tools to maximize impact of electronic/internet/social media tools**

## **Remodel external LANL.gov website**

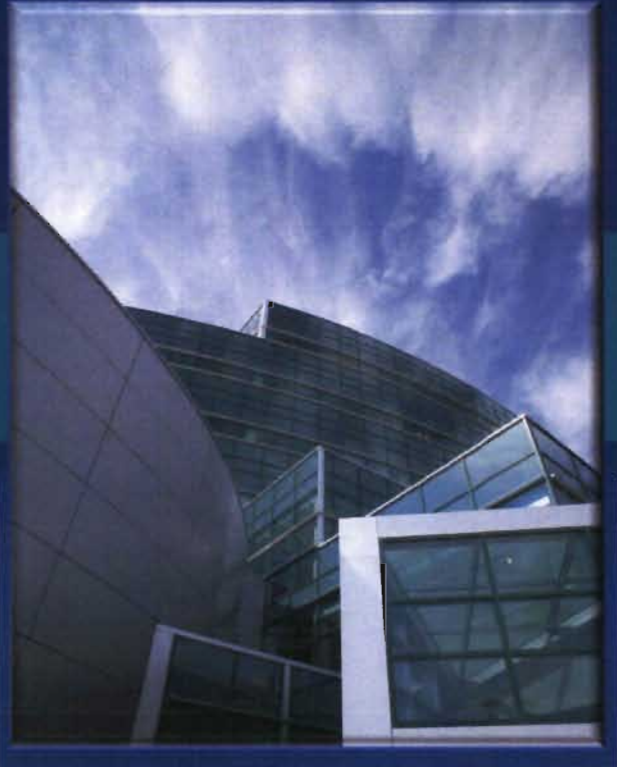
## **Restructure internal LANL website for content management system**



LANL's new social media icon for  
Flickr, YouTube, Twitter, LinkedIn,  
iTunes, and Facebook posts

*Communications initiative established at November 2011 off-site  
by the LANL senior management team*





# Supplementary Material

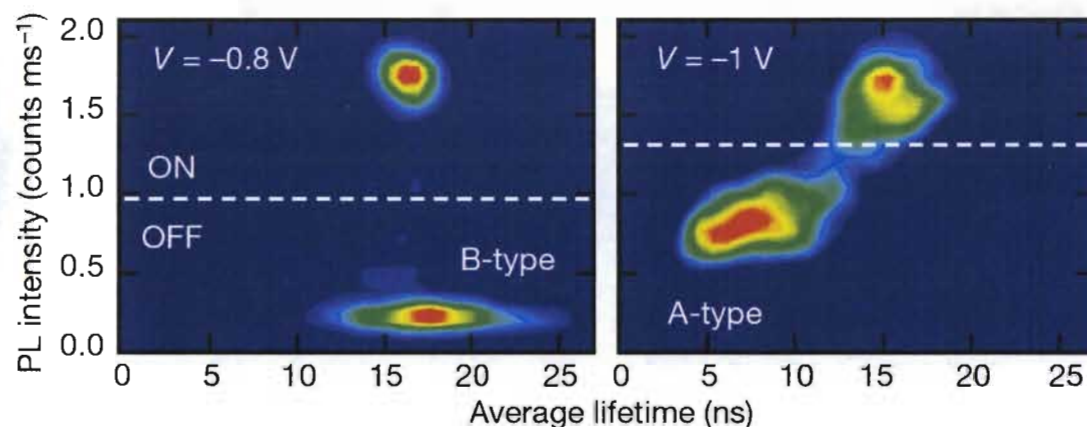
## Energy Security mission:

Scientists control the undesirable blinking of quantum dots

**Revealed two different, controllable “blinking” mechanisms for quantum dots. (*Nature*, 2011)**

- Conventional (A-type) blinking is due to charging and discharging of the nanocrystal core.
- B-type blinking is due to charge fluctuations in the electron-accepting surface sites.

**Determined that blinking can be controlled—and even completely suppressed—electrochemically.**



*Electrochemically controlled switching in one nanocrystal.  
B-type blinking at -0.8V (left); A-type blinking at -1V (right).*



*Understanding how to suppress the blinking could lead to applications for solid state lighting, light-emitting diodes, single-photon sources, and highly efficient solar cells.*



# Global Security & Energy Security missions: Developed method to control cushioned biomembranes

*Provides a simple means to control the biomembrane architecture and its properties.*

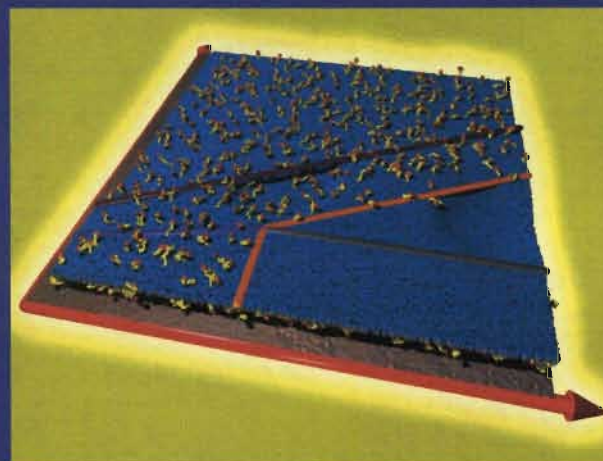
Lujan Center's SPEAR enables examination of the membrane's structure.

By controlling the interaction energy of the polymer with the underlying surface, the membrane can

- Float on top of a well-anchored polymer cushion,
- Rearrange to expose a polymer chain forest to the environment
- Create a hybrid system where the membrane is decorated on both sides with the polymer chains

**Langmuir**  
The ACS Journal of Surfaces and Colloids

NOVEMBER 15, 2011  
VOLUME 27, NUMBER 22  
[pubs.acs.org/Langmuir](http://pubs.acs.org/Langmuir)



**Biomembrane Cushions: Novel Architectures of  
Polymer Decorated Lipid Bilayers**

(see p. 5A)

ACS Publications  
MOST TRUSTED. MOST CITED. MOST READ.

[www.acs.org](http://www.acs.org)

*Phase diagram for polymer-decorated lipids  
embedded in a biomembrane*

LA-UR-12-00XXX: 44

# Strategic Science PBIs: FY12/Q1 Progress

## **PBI 9: Excellence in Scientific and Programmatic Pursuits (\$4.5M Subjective)**

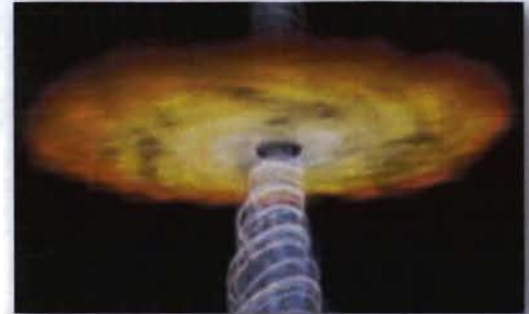
### **9.7 National Security Science Laboratory**

LDRD: FY12 Plan approved

Facility revitalization execution underway

### **9.8 Energy Security**

Conducted deep dives in three focus areas to guide FY12 mission execution and growth



## **PBI 11: Excellence in Business and Institutional Management (\$6.7M Subjective)**

### **11.9 Work for Others Integration and Execution**

Progress underway



## **PBI 12: Award Term Measures**

### **12.5 Science of Signatures in Nuclear/Radiological and Sensing/Measurement**

Progress underway

