

FY2012 Performance Evaluation and Measurement Plan

End of Year Report

Submitted: October 1, 2012

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## **PREFACE**

In December, 2006, Iowa State University and DOE entered into a new M&O contract DE-AC02-07CH11358 for the period December 4, 2006 through December 31, 2011; subsequent Mods extended the period of performance through December 31, 2015, and additional one year extension has been earned that has not yet been documented in a Mod. Under the terms in this contract, specifically Clause H.25 and I.96, the Parties agreed to utilize a performance-based management system for Laboratory oversight, and ISU, as the contractor, is required to provide a written assessment of the Contractor's and Laboratory's performance. The purpose of a performance-based management system is to encourage and reward excellence, continuous improvements and timely communication. Appendix B, to the Contract, Modification M105, provided the objectives, measures and expectations for fiscal year 2012.

This report contains the end of year status for each of the objectives and covers the period October 1, 2011–September 30, 2012.

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## INTRODUCTION

This document, the Performance Evaluation and Measurement Plan (PEMP), primarily serves as DOE's Quality Assurance/Surveillance Plan (QASP) for the evaluation of Iowa State University (hereafter referred to as "the Contractor") performance regarding the management and operations of the Ames Laboratory (hereafter referred to as "the Laboratory") for the evaluation period from October 1, 2011, through September 30, 2012. The performance evaluation provides a standard by which to determine whether the Contractor is managerially and operationally in control of the Laboratory and is meeting the mission requirement and performance expectations/objectives of the Department as stipulated within this contract.

This document also helps determine the Contractor's fee for the management and operation of the Laboratory during FY2012. In partnership with the Contractor and other key customers, the Department of Energy (DOE) Headquarters (HQ) and the Site Office have defined the measurement basis that serves as the Contractor's performance-based evaluation and fee determination.

The Performance Goals (hereafter referred to as Goals), Performance Objectives (hereafter referred to as Objectives) and set of Performance Measures and set of Notable Outcomes (Performance Measures/Targets) discussed herein were developed in accordance with contract expectations set forth within the contract. The Notable Outcomes for meeting the Objectives set forth within this plan have been developed in coordination with HQ program offices as appropriate. Except as otherwise provided for within the contract, the evaluation and fee determination will rest solely on the Contractor's performance within the Performance Goals and Objectives set forth within this plan.

Complete details on the determination/assessment of objective ratings can be found in Mod 105 to Contract DE-AC02-07CH11358.

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## EXECUTIVE SUMMARY

Fiscal year 2012 began and ended with a flurry of research, planning and technology transfer activities.

The national and international focus on rare earths continues to bring potential partners to the Laboratory.

Highlights include:

- NOVA, the PBS television series, featured the lanthanides in their April 4, 2012 program about “The Elements”. Included was the Ames Laboratory's Materials Preparation Center.
- As part of our signature Materials Discovery and Design efforts that promote integrated theory and experiment materials development for impact in societal use, we were awarded ARPA-E funding for two REACT projects involving computationally-driven design/synthesis of rare earths and permanent magnets; *"Novel High Energy Permanent Magnet without Critical Elements"* led by AMES and *"Development of MnBi/Al Based Permanent Magnet with 40 MGOe at 200°C"* led by PNNL with Ames.
- Bill McCallum was featured in a National Geographic Article entitled “While Rare-Earth Trade Dispute Heats Up, Scientists Seek Alternatives”. The story is part of a special series that explores energy issues.
- With the support of our Contractor, ISU, a new Materials Sciences and Engineering (MSE) course in Rare Earths was offered this Spring semester and taught by an Ames Laboratory scientist.
- Again, as part of our signature Materials Design efforts, and at ARPA-E’s suggestion from a well-reviewed REACT proposal in 2011, we submitted in July to ARPA-E FCE open call a proposal entitled *“Solid State Processing of Fully Dense Anisotropic Nanocomposite Magnets”*.
- A visiting scientist from South Korea’s KITECH started in April to develop a report on strategic areas in rare-earth research. A CRADA is also being negotiated to support this work.
- The Ames Laboratory received visitors from companies, universities and not for profits as well as government officials in 2012 to discuss rare earth research and rare earth business sensitive issues. Most of these visits were covered under individual non-disclosure agreements.
- The Ames Laboratory developed several new strategic partnerships with leading U.S. industries in the critical rare-earth recycling and re-use arenas, including Advanced Recovery, Cytec Industries, GE Global Research, Molycorp, OLI Systems, Inc., Simbol Materials, as well as three National Laboratories with separations and advanced manufacturing facilities – INL, ORNL, and LLNL. From this one-and-half-year activity, the Ames Laboratory led a proposal submitted in August, 2012 to EERE for a Critical Materials Hub.
- An offer was made (details under negotiation) to an internationally recognized rare-earth scientist to enhance laboratory capabilities and address our succession and diversity planning.

Other scientific highlights in 2012 include:

- Danny Shechtman won the 2012 Nobel Prize in Chemistry for the discovery of quasicrystals. What makes this significant is the research at the Ames Laboratory, with DOE funding, that helped to verify Dr. Shechtman’s finding.
- Robert McQueeney became a part-time detailee in Washington for BES scattering sciences and DOE has extended the detail for another year.
- An Americas Next Top Energy Innovator optionee (IPAT) won the DOE’s ANTEI challenge for titanium powder atomization. IPAT was also awarded first prize in the 2012 John Pappajohn Iowa Business Plan Competition, announced September 27, 2012.
- Paul Canfield won the DOE Ernest Orlando Lawrence Award.

- New superconducting materials were made to behave in two distinct ways, helping break down a significant barrier to understanding the mechanisms of high-temperature superconductivity. Known high temperature superconductors fall into two different classes – layered cuprates and iron arsenides.
- High-level, quantum chemistry *ab initio* calculations for critical water chemistry simulations (1000+ molecules) were demonstrated, via an INCITE grant at Argonne, to scale nearly linearly on 100,000+ cores on a Blue Gene/P computer with new algorithms, reducing compute time to less than 7 minutes.
- Researchers showed how to probe a catalyst's inner workings making direct optimization now realizable. This was made possible by new solid-state nuclear magnetic resonance (SS-NMR) methods and by innovative synthetic strategies on bound catalysts.
- Researchers used a combined experimental and theoretical approach to show that precursor reactivity determines the relative ease of formation of different nanocrystals. Specifically, photocatalysts made from tiny amounts of cadmium, sulfur and selenium will form selectively into shapes that look like either tadpoles or drumsticks depending on the relative reactivity of the selenium and sulfur precursors.
- Researchers attacked a significant problem for further development of IMAGETags. The problem is related to the nature of the ligand. The ligand needs to be able to readily penetrate the cell and also should not bind tightly to any cellular component. As a first step in this direction, we took a combinatorial approach in conjunction our SFA co-workers at LBNL to develop a ligand that has low retention in the cells. This ligand will be used to develop an aptamer that will then be incorporated into IMAGETags.
- Researchers developed a new software algorithm for self-calibration of metal fracture (toolmarks) characterization and matching that improves the confidence level of such matching at multiple-length scales. The new method, funded by the National Institute of Justice, yields a greatly improved understanding and confidence in this key type of forensic evidence, frequently encountered in criminal cases.
- To enhance SS-NMR capabilities, begin implementation of our Center for Solid State NMR Science initiative, and impact our signature Catalysis, and Materials Discovery and Design efforts, the Ames Laboratory and PNNL jointly held an international conference on "Challenges for Advanced Nuclear Magnetic Resonance" 7-9 December 2011. The purpose was to assess new directions and the potential for high-resolution Dynamic-Nuclear-Polarization NMR to provide unparalleled resolution of chemical reactions. First data from DNP-NMR experiments on mesoporous catalysts were performed in collaboration with researchers in Switzerland and France in the summer of 2012 showed a remarkable increase in resolution for catalytic reactions (publications in preparation).
- The Laboratory awaits delivery of two key computer clusters to support our signature efforts in Materials Design and Design of Metamaterials, see Section 3.2 for full details. For materials design, with half of the cost from a DOE mid-year equipment request, we have ordered a \$972K HPC cluster based on low-energy Intel chips for lower operational costs. For design of anisotropic metamaterials and plasmonic nanostructures, a second 8-node, very large-memory computer was funded by BES mid-year equipment request.

For additional information on our scientific impact in 2012, see Goals 1.0 and 3.0.

Management, facilities, and operations highlights include:

- There were no recordable injuries or DART cases in FY2012 to date, and only six first aid cases.
- Diversity of applicants improved in our pools for open positions as a result of targeted advertisements.
- The Associate Laboratory Director participated on the Committee to get the Accelerated Commercialization of Technologies (ACT) Agreement accepted and we are one of the 9 pilot labs.
- Progress was made on the Sensitive Instrument Facility, identified in the 2011 Lab Plan as one of our critical facilities and infrastructure projects needed to support Laboratory missions and programs.

Funding totaling \$5.5M has been received from the Office of Science for the project. The Site Evaluation Study by outside consultants has been completed and the procurement of A/E design services is complete. The Laboratory has received its first deliverable from A/E, the Program Report, and they are working on the next set of deliverables.

- Ames Laboratory developed technologies generated \$9,174,898 in royalty income from inventions in Fiscal Year 2011, based on \$766,879,618 in sales. As estimated from the EOY budget, we expect royalty income for 2012 to be near the 2011 level.
  - Of those sales, \$110,641,350 were from Iowa-based companies, and these sales support more than 540 jobs in the manufacturing sector.
  - The total represents over \$22 of economic activity for every dollar spent by the Laboratory.
- The Spedding Auditorium renovation was completed in FY2012. This facility has extensive A/V, networking, and distance learning capability, providing modern and flexible conferencing, scientific review and meeting space. The new facility presents an excellent image of the Laboratory to visitors and staff. It was used for the first time for the visit of Deputy Secretary of Energy Poneman and, most recently, for the BES/MSED Laboratory Management review on September 17 via televideoconference to Germantown, saving significant travel costs.
- We have continued to strategically increase our post-doctoral salaries to become more competitive with sister DOE laboratories, and improve the draw of highly capable talent to the Ames Laboratory.
- In consultation with ISU and AMSO, the Laboratory determined two opportunities for improvement to our Contractor Assurance System that will provide the most cost-benefit; namely, identify our most pressing risks, and identify the most useful metrics to use as key indicators.
- Negotiated procurement actions provided over \$300,000 in cost savings..
- The relining half of the fume hood stacks in Spedding Hall was completed. This resulted in a sizable reduction in the amount of air moving through the stacks. The Facilities and Engineering Services group anticipates that this could reduce our heating costs by approximately 10%.

From our 2012 Goals and Objectives we have ranked our achievements as follows:

| Goal/Objective/Notable Outcome  | Grade<br>(> or < B+) |
|---|----------------------|
| Goal 1. Provide for Efficient and Effective Mission Accomplishment.   | A                    |
| 1.1 Provide Science and Technology Results with Meaningful Impact on the Field.                                       | A                    |
| 1.2 Provide Quality Leadership in Science and Technology that Advances Community Goals and DOE Mission Goals.         | A                    |
| Goal 3. Provide Effective and Efficient Science and Technology Program Management.                                    | A                    |
| 3.1 Provide Effective and Efficient Strategic Planning and Stewardship of Scientific Capabilities and Program Vision. | A                    |

| <b>Goal/Objective/Notable Outcome</b>   | <b>Grade<br/>(&gt; or &lt; B+)</b> |
|---|------------------------------------|
| 3.2 Provide Effective and Efficient Science and Technology Project/Program/Facilities Management.   | A-                                 |
| 3.3 Provide Efficient and Effective Communications and Responsiveness to Headquarters Needs.  | A                                  |
| <b>Notable Outcome 3A (BES).</b> Refined the strategic vision for, and continue execution of, a signature effort on materials discovery and design.             | Met                                |
| <b>Goal 4. Provide Sound and Competent Leadership and Stewardship of the Laboratory.</b>  | A-                                 |
| 4.1 Leadership and Stewardship of the Laboratory.   | A-                                 |
| 4.2 Management and Operation of the Laboratory.   | B+                                 |
| 4.3 Contractor Value-added.   | A-                                 |
| <b>Notable Outcome 4A.</b> Host a contractor Assurance System (CAS) Peer Review.  | Met                                |
| <b>Goal 5. Sustain Excellence and Enhance Effectiveness of Integrated Safety, Health and Environmental Protection.</b>  | A-                                 |
| 5.1 Provide an Efficient Worker Health and Safety Program.  | A                                  |
| 5.2 Provide Efficient and Effective Environmental Management System.  | B+                                 |
| <b>Goal 6. Deliver Efficient, Effective, and Responsive Business Systems and Resources that Enable the Successful Achievement of the Laboratory Mission(s).</b> | B+                                 |
| 6.1 Provide an Efficient, Effective, and Responsive Financial Management System(s).   | B+                                 |
| 6.2 Provide an Efficient, Effective, and Responsive Acquisition Management System.  | B+                                 |
| 6.3 Provide an Efficient, Effective, and Responsive Property Management System.   | B+                                 |
| 6.4 Provide an Efficient, Effective, and Responsive Human Resources Management System and Diversity Program.  | A-                                 |

| <b>Goal/Objective/Notable Outcome</b>   | <b>Grade<br/>(&gt; or &lt; B+)</b> |
|---|------------------------------------|
| 6.5 Provide Efficient, Effective, and Responsive Management Systems for Internal Audit and Oversight; Quality; Information Management; Assurance System and Other Administrative Support Services as Appropriate.   | B+                                 |
| 6.6 Demonstrate Effective Transfer of Technology and Commercialization of Intellectual Assets.  | A-                                 |
| <b>Notable Outcome 6A.</b> Ames Laboratory subject matter experts for Work For Others (WFO), Intellectual Property (IP), Cyber Security, Safeguards & Security (S&S) and Science will work together to develop an integrated plan to address potentially sensitive information developed during scientific research, including WFO. | Met                                |
| <b>Notable Outcome 6B.</b> Implement planned improvements resulting from the proposal submission improvement process review committee conducted during FY2011. Areas of emphasis should include timeliness and quality of packages sent to DOE.   | Met                                |
| <b>Goal 7. Sustain Excellence in Operating, maintaining, and Renewing the Facility and Infrastructure Portfolio to Meet Laboratory Needs</b>  | B+                                 |
| 7.1 Manage Facilities and Infrastructure in an Efficient and Effective Manner that Optimizes Usage, Minimizes Life Cycle Costs, and Ensures Site Capability to Meet Mission Needs.  | B+                                 |
| 7.2 Provide Planning for and Acquire the Facilities and Infrastructure Required to Support the Continuation and Growth of Laboratory Missions and Programs.   | B+                                 |
| <b>Notable Outcome 7A.</b> The Mission Readiness Leadership Team will prepare a written evaluation of the review team's opportunities for improvement, including a plan of action for those recommendations deemed beneficial to implement.   | Met                                |
| <b>Goal 8. Sustain and Enhance the Effectiveness of Integrated Safeguards and Security Management (ISSM) and Emergency management Systems</b>   | A-                                 |
| 8.1 Provide an Efficient and Effective Emergency Management System.   | A-                                 |
| 8.2 Provide an Efficient and Effective System for Cyber-Security and National Security Systems (NSS).   | B+                                 |

| <b>Goal/Objective/Notable Outcome</b>   | <b>Grade<br/>(&gt; or &lt; B+)</b> |
|---|------------------------------------|
| 8.3 Provide an Efficient and Effective System for the Physical Security and Protection of Special Nuclear Materials, Classified Matter, and Property.   | A-                                 |
| 8.4 Provide an Efficient and Effective System for the Protection of Classified and Sensitive Information.   | B+                                 |
| Notable Outcome 8A. Once the PCSP is released, complete a plan for transition of the security authorization to the risk management framework, establish milestones for implementation, and complete milestones that fall within FY2012. | Met                                |

## PERFORMANCE GOALS, OBJECTIVES & NOTABLE OUTCOMES

### Background

The current performance-based management approach to oversight within DOE has established a new culture within the Department with emphasis on the customer-supplier partnership between DOE and the laboratory contractors. It has also placed a greater focus on mission performance, best business practices, cost management, and improved contractor accountability. Under the performance-based management system the DOE provides clear direction to the laboratories and develops annual performance plans (such as this one) to assess the contractors performance in meeting that direction in accordance with contract requirements. The DOE policy for implementing performance-based management includes the following guiding principles:

1. Performance objectives are established in partnership with affected organizations and are directly aligned to the DOE strategic goals;
2. Resource decisions and budget requests are tied to results; and
3. Results are used for management information, establishing accountability, and driving long-term improvements.

The performance-based approach focuses the evaluation of the Contractor's performance against these Performance Goals. Progress against these Goals is measured through the use of a set of Objectives. The success of each Objective will be measured based on a set of Notable Outcomes, both objective and subjective, that are to focus primarily on end-results or impact and not on processes or activities. Measures provide specific evidence of performance, and collectively, they provide the body of evidence that indicates performance relative to the corresponding Objectives. On occasion however, it may be necessary to include a process/activity-oriented measure when there is a need for the Contractor to develop a system or process that does not currently exist but will be of significant importance to the DOE and the Laboratory when completed or that lead to the desired outcome/result.

The information in the following sections summarizes the Laboratory's performance for FY2012.

## Goal 1.0 Provide for Efficient and Effective Mission Accomplishment

### Highlights by Objective:

#### 1.1 Provide Science and Technology Results with Meaningful Impact on the Field

The following Ames highlights have been submitted to DOE throughout the course of the FY2012: (Note: For further information on these highlights, please go to [www.ameslab.gov/research/highlights](http://www.ameslab.gov/research/highlights)).

- **Properties of Magnets Explained**

A new theoretical advance enables us to understand how the magnetic properties of a class of magnets called antiferromagnets respond to a magnetic field. The theory describes the magnetic behaviors of both collinear antiferromagnets, in which adjacent magnetic moments point in opposite directions from atom-to-atom, and noncollinear antiferromagnets, where the magnetic moments rotate from one atom to the next. Advantages of this theory include that it is expressed in quantities that are easily measurable and is useful for polycrystalline samples. Applications of the theory to specific compounds illustrate its general utility to understand the properties of antiferromagnets. This theory will help us to understand the interactions between atomic magnets needed for the development of new magnetic materials for such applications as computers, electric motors and other devices that we extensively use in our everyday lives.

- **Dramatic Efficiency Improvements for Organic Light Emitting Diodes**

Significant LED performance improvements have been achieved by taking advantage of novel materials. An organic light emitting diode (OLED) requires at least one transparent electrode, which is most commonly indium tin oxide (ITO). While ITO is both transparent and a good electrical conductor, its light transmission differs from the other organic material layers used in the device, thereby leading to internal reflections which reduce efficiency. Researchers replaced ITO with a special highly conductive polymer known as PEDOT: PSS. The new OLEDs have a peak power efficiency and other key properties that are among the highest reported to date. They are 44% more efficient than comparable devices made with ITO. The researchers used computer simulations to show that the enhanced performance is largely an effect of the difference of optical properties between the polymer-based electrode and ITO. Because of the improved efficiency and potentially easier processing of these ITO-free OLEDs, the results pave the way for improved commercial OLEDs at lower cost.

- **Cooperative Catalyst leads to Transformative Results**

Capitalizing on the concept that everything proceeds faster with a little cooperation, researchers showed how designing cooperation into solid catalysts leads to enormous benefits. Catalysts attached to a porous solid support are preferred industrially because they are easier to separate from liquid products and reuse. But, these bound catalysts typically do not perform as well and probing their interiors to figure out how to improve them has proved difficult until now. Using new solid-state nuclear magnetic resonance (SS-NMR) methods (the equivalent of running an MRI on the catalyst) and innovative synthetic strategies, researchers showed how to probe their inner workings and make optimization possible. Scientists demonstrated this approach on a carbon-carbon bond forming reaction routinely used in chemical manufacturing and biofuel production. Two key insights were revealed. First, access into and out of the pores is blocked by a chemical intermediate. Making the pores a mere 0.8 nanometers wider increased the catalytic activity 20-fold! Knowing the structure of the intermediate, researchers were able to modify the catalyst to eliminate the bottleneck without making the pore wider. This heterogeneous catalyst is significantly more active than the homogeneous catalysts, contrary to expectations. Why? SSNMR showed the support brings the reactants and catalytic groups together, resulting in the enhanced, cooperative activity not possible with the



untethered catalyst. This work sets the stage for significant innovations for commonly used catalytic processes.

- **Decades-Long Mystery Solved**

Scientists have helped solve an 80-year-old puzzle about a widely used chemical process. The Fenton reaction involves iron and hydrogen peroxide and is used to treat wastewater worldwide. Does the reaction involve a radical intermediate? Or, is it the non-radical, iron species known as Fe(IV)? The exact nature of the intermediate has been debated for decades with data to support both theories. The problem is both intermediates will react to form the same products in most cases making the reaction intermediate hard to pin down. Researchers have now proved that both intermediates can be involved — it just depends on the pH. They carefully studied a reaction for which the two intermediates would form different products. They showed that in an acidic environment, the intermediate is an hydroxyl radical, whereas at near neutral pH the intermediate is Fe(IV). This discovery explains the differences in products formed under certain reaction conditions and clears up a decades-old mystery.

- **Rare Earth makes the Best Better**

One of the best materials for converting heat to electricity just got 15% better. Adding a small amount of dysprosium to the thermoelectric known as TAGS-85 raises the thermoelectric figure of merit from 1.3 to 1.5. Researchers examined the mechanism by which doping with dysprosium affects the thermopower. The size of dysprosium along with its local magnetic characteristics modifies the interplay between electronic and thermal transport. Dysprosium distorts the local crystalline lattice and enables higher energy carriers to move preferentially through the material. This leads to improved heat conversion. Understanding how doping impacts thermoelectric properties will help researchers design even better thermoelectric materials. An improvement of 0.2 in the figure of merit is a big step toward the goal of 2.0, which is regarded as the requirement for the commercialization of thermoelectric power generation.

- **What Makes a High-temperature Superconductor a Superconductor?**

Researchers may have discovered the key to high temperature superconductivity — quantum criticality. A quantum critical point occurs where a material undergoes a continuous transformation at absolute zero. For superconducting cuprates and iron-arsenides, the curve of the superconducting transition temperature,  $T_c$ , versus doping (or pressure) is dome shaped. It wasn't clear until now if superconductivity prevents a quantum critical point or if quantum critical behavior is hidden beneath the dome. An international team studied a barium-iron arsenic superconductor where arsenic is partially substituted with phosphorous,  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ . Phosphorous substitution suppresses magnetism and induces superconductivity leading to a maximum  $T_c$  when magnetism is fully suppressed. The team measured the characteristic decay of the magnetic field at the surface, the so-called London penetration depth, and found quantum critical behavior coexists with and may actually be protected by superconductivity. Better understanding what drives high temperature superconductivity will accelerate the search for new, higher temperature superconductors.

- **Warning: Single Lane Tunnel Ahead**

A new theory shows that reactivity at catalytic sites inside narrow pores is controlled by how molecules move at the pore openings. Like cars approaching a single lane tunnel from which other cars are emerging, the movement of molecules depends on their distance into the pore; near the ends of the pores, exchange is rapid compared to further into the pores. Dynamics at the openings of these pores controls the penetration of reactants and thus overall conversion to products. Overall, the behavior of catalytic reactions in narrow pores is controlled by a delicate interplay between fluctuations at pore openings, restricted diffusion, and reaction. Until now it has been impossible to reconcile analytical theories with the findings of detailed step-by-step simulations. The new theory enables calculations of reactant and product distributions in minutes

compared to the hours or days it takes to do the detailed simulations and yields comparable results. Thus, this new theory is a powerful tool for analyzing the catalytic behavior in these systems.

- **Finding Order amid the Chaos**

Glass is often described as being like a liquid, with randomly arranged atoms. New insights are emerging that show some distinct levels of order within the structure of glasses. Our rapidly evolving understanding arises from new structural information made possible because of advanced light sources like the U.S. Department of Energy's Advanced Photon Source. The new theory fits experimental data better than the widely accepted model based on icosahedral-like clusters. The new model shows many crystal-like polyhedra as well as clustering of polyhedra — features not seen in previous models. Similar clusters group together into nanometer sized regions. The structure emerges by linking short range effects determined from the forces acting on each atom, with medium range information from electron microscopy. After heating for long periods of time to encourage structural relaxation, glasses increasingly conform to the older model suggesting that this represents an ideal glass. Practical glasses that are not heated for so long have more complex structures. This has important implications for designing and manufacturing metallic glasses.

- **Follow the Light**

Just like watching boats in the night, seeing movement at the nanoscale is easier when the object you are watching has a beacon. Dynamic three-dimensional tracking with high precision is possible with nanoscale light emitting particles known as quantum dots at better resolution than 10 nanometers in the vertical direction. This opens up the possibility for understanding three dimensional movements in nanoscale structures and biological systems. The quantum dots are followed using the technique known as scanning-angle total internal reflection fluorescence microscopy (SA-TIRFM). Quantum dots hold advantages over other fluorescent probes because they can be tuned to emit various colors of light. Many, however, will spontaneously “blink” meaning the emitted light is suddenly turns off (or on) thus interrupting measurements. Researchers have developed “non-blinking” quantum dots that make them useful for high precision tracking in dynamic environments. This methodology was used to show the potential of motor proteins as components in nanomachines to transport cargo.

- **Manipulating Light with a Single Layer of Carbon**

Researchers have shown that it may be possible to make lasers using single-layer sheets of carbon atoms — the novel material known as graphene. Lasers are made from materials that can absorb ordinary light and then emit photons that have matching waves to provide high intensity. To generate laser power, a material must first undergo a population inversion where an excess of electrons is excited. They must then produce optical gain when one photon is emitted spontaneously causing the excited state electrons to undergo a cascade reaction, each one emitting an additional photon coherent with the first, so a large intensity builds up. Graphene exhibits both of these properties. Very short light pulses, only a few femtoseconds (10-15 seconds) in duration, were used to stimulate the graphene. Almost instantaneously broad population inversions were observed; and the ultrabroad band gain is established at about 10 femtoseconds, producing a much wider tuning range of light (from terahertz to ultraviolet) than in conventional lasing materials. This is remarkable for photonics materials. Comparison of the experiments with newly-developed theoretical approaches neatly explains the findings. This work opens up a wide range of possible uses of graphene in previously-unexplored areas, particularly ultra-fast telecommunications and laser technology. With graphene a little light may go a long way.

- **Pick a Material, Not just Any Material, for a Metamaterial**

Designing the building blocks of artificially engineered materials, known as metamaterials, just got easier. Metamaterials are built from small engineered structures that, in some ways, mimic the role of atoms, and

can manipulate light in ways not seen in nature. The conducting materials used to make them are central to their efficiency. Energy is lost by conversion of light to heat in the metallic components and the support materials. Gold and silver are known to be relatively good building block materials and now we have a way to predict which other materials could work even better. Materials with a lower optical resistivity at the wavelength of the light are key, but geometry has an effect too. For example, graphene, one atomic layer thick graphite, would work well if not for being unobtainable at greater thicknesses. Superconductors may also have merit, although their properties are entirely different. This work provides a tool to select materials with optimum optical properties for use in metamaterials. The potential impact could be huge, because of the considerable efficiency improvements that are possible.

- **Making Maps of the Molecules in Seeds**

Scientists have advanced methods to make maps of the locations of molecules within plant materials. Resolution of 10 to 50 microns, less than a quarter the size of a human hair, is routinely possible. The trick with plant materials is to extract the molecules delicately from thin slices with a fine laser moving stepwise across the sample. Many molecules are analyzed at once using a very sensitive mass spectrometer in this technique known as matrix-assisted laser deposition/ionization-mass spectrometry imaging (MALDI-MS). Within cottonseed embryos, which are about 3/16th of an inch in diameter, this method showed a surprisingly non-uniform mixture of lipids whose concentration varies with tissue functionality. These lipids are important for seed development and can affect the chemistry of the cottonseed oil extracted for use in various foods. These findings demonstrate the potential of this technique to provide a new level of understanding of biosynthetic pathways.

- **Ultrafast Moves – Caterpillar Style**

A layer of lead on clean silicon moves in a surprising way — in waves like a caterpillar. This explains the unexpected ultrafast mass transport observed even at low temperatures for this system. Although solid these single layers of atoms move as fast as molten lead. Computer simulations show that the lead layer forms waves that require almost no energy to keep moving thus explaining the quickness of mass transport. Other metals on surfaces typically move much slower by one atom at a time hopping along the surface. Knowing the critical parameters that give rise to this cooperative liquid-like movement, other systems may be discovered that move the same way and this could have important implications for applications requiring ultrathin films.

- **Rounding Corners to Make Superconductors Work Better**

Making superconducting nanocircuits with rounded internal corners will significantly improve performance. Scientists showed this by calculating how circuit geometry impacts current flow. The key is how geometry affects “current crowding”. Crowding can happen when electrical current travels around a sharp corner or hairpin turn much like cars racing on a tight track. The current (like cars) tends to concentrate near the inner edges of sharp turns. By rounding the corners this bottleneck is eased. This work explains reduced critical currents observed in manufactured devices and has important implications for both superconducting and metal film devices, including nanowire single photon detectors and devices that measure extremely small magnetic fields.

- **Expulsion Leads to a New Catalyst**

Locating a catalyst and reactants in confined spaces makes catalytic reactions go faster in the desired direction. Of course, the reaction products have to be removed from the confined spaces and researchers have developed a new approach to expelling aqueous reaction products. This works for confinement in nanometer-sized pores in silica particles. By lining the insides of the pores with both catalysts and a fluorinated chemical, like that found in Teflon®, reactions with water as a byproduct proceed much faster.

This works because certain chemicals just don't like each other. Oil and water tend to separate. Water on a Teflon<sup>®</sup>-coated frying pan balls up to minimize its contact with the Teflon<sup>®</sup>. Combining state-of-the-art characterization and theory, a structure was designed to maximize this effect inside the catalytic pores. The performance of this catalyst surpasses the commercially available ones for a reaction known as esterification, which yields water as a byproduct. This is the first demonstration of enhancing chemical transformations by expelling the byproducts from porous catalytic materials in this manner and just the beginning of essentially a new class of catalysts.

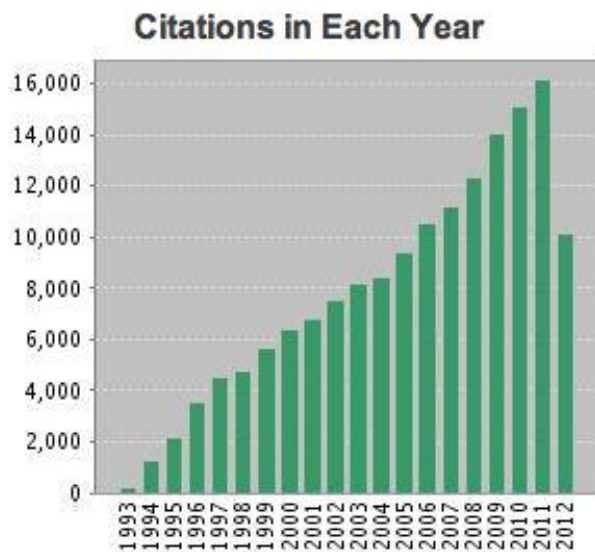
Based upon the above information, the Laboratory assesses its Science and Technology Results with Meaningful Impact as an A.

## 1.2 Provide Quality Leadership in Science and Technology that Advances Community Goals and DOE Mission Goals

### Overall Statistics

As of 9/24/12, published 271 papers for FY2012 according to ISI Web of Science:

- 60% involved collaborations with researchers not from Ames Laboratory or ISU
- 36% involved international collaborations with, in total, 27 different countries.
- 4% (12) very high impact peer-reviewed journal articles (impact factor > 10)
- 9% (24) high impact peer-reviewed journal articles (impact factor  $6 < x < 10$ )
- 13% involved work with other National Laboratory researchers
- 7 Special editor's selected papers
- 3 journal covers (Israel Journal of Chemistry, Chemical Communications, and Zeitschrift für Anorganische und Allgemeine Chemie)



Citations for paper published from CY1993 – present sorted by year cited as of 9/18/12 according to ISI Web of Science

## Journal Articles:

### ○ Top Five most Cited Papers Published in FY2012 and Cited in FY2012

M. S. Gordon, D. G. Fedorov, S. R. Pruitt and L. V. Slipchenko "Fragmentation Methods: A Route to Accurate Calculations on Large Systems" *Chemical Reviews*, 2012, 112, 632-672. DOI 10.1021/cr200093j Cited 25 times.

R. M. Fernandes, E. Abrahams and J. Schmalian "Anisotropic In-Plane Resistivity in the Nematic Phase of the Iron Pnictides" *Physical Review Letters*, 2011, 107, 217002. DOI 10.1103/PhysRevLett.107.217002 Cited 13 times.

A. Pandey, R. S. Dhaka, J. Lamsal, Y. Lee, V. K. Anand, A. Kreyssig, T. W. Heitmann, R. J. McQueeney, A. I. Goldman, B. N. Harmon, A. Kaminski and D. C. Johnston " $Ba_{1-x}K_xMn_2As_2$ : An Antiferromagnetic Local-Moment Metal" *Physical Review Letters*, 2012, 108, 087005. DOI 10.1103/PhysRevLett.108.087005 Cited 8 times.

L. N. Bulaevskii, M. J. Graf and V. G. Kogan "Vortex-assisted photon counts and their magnetic field dependence in single-photon superconducting detectors" *Physical Review B*, 2012, 85, 014505. DOI 10.1103/PhysRevB.85.014505 Cited 7 times.

R. S. Dhaka, C. Liu, R. M. Fernandes, R. Jiang, C. P. Strehlow, T. Kondo, A. Thaler, J. Schmalian, S. L. Bud'ko, P. C. Canfield and A. Kaminski "What Controls the Phase Diagram and Superconductivity in Ru-Substituted  $BaFe_2As_2$ ?" *Physical Review Letters*, 2011, 107, 267002. DOI 10.1103/PhysRevLett.107.267002 Cited 7 times.

### ○ Top Ten Most Cited Papers Published in the Last 5 Years (2008-Present)

C. de la Cruz, Q. Huang, J. W. Lynn, J. Y. Li, W. Ratcliff, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang and P. C. Dai "Magnetic order close to superconductivity in the iron-based layered  $LaO_{1-x}F_xFeAs$  systems" *Nature*, 2008, 453, 899-902. DOI 10.1038/nature07057 Cited 905 times.

N. Ni, S. L. Bud'ko, A. Kreyssig, S. Nandi, G. E. Rustan, A. I. Goldman, S. Gupta, J. D. Corbett, A. Kracher and P. C. Canfield "Anisotropic thermodynamic and transport properties of single-crystalline  $Ba_{1-x}K_xFe_2As_2$  ( $x=0$  and  $0.45$ )" *Physical Review B*, 2008, 78, 014507. DOI 10.1103/PhysRevB.78.014507 Cited 377 times.

I. I. Slowing, J. L. Vivero-Escoto, C. W. Wu and V. S. Y. Lin "Mesoporous silica nanoparticles as controlled release drug delivery and gene transfection carriers" *Advanced Drug Delivery Reviews*, 2008, 60, 1278-1288. DOI 10.1016/j.addr.2008.03.012 Cited 320 times.

D. C. Johnston "The puzzle of high temperature superconductivity in layered iron pnictides and chalcogenides" *Advances in Physics*, 2010, 59, 803-1061. DOI 10.1080/00018732.2010.513480 Cited 277 times.

M. S. Torikachvili, S. L. Bud'ko, N. Ni and P. C. Canfield "Pressure induced superconductivity in  $CaFe_2As_2$ " *Physical Review Letters*, 2008, 101, 057006. DOI 10.1103/PhysRevLett.101.057006 Cited: 255 times

K. Schmidt-Rohr and Q. Chen "Parallel cylindrical water nanochannels in Nafion fuel-cell membranes" *Nature Materials*, 2008, 7, 75-83. DOI 10.1038/nmat2074 Cited: 245 times

T. Kondo, A. F. Santander-Syro, O. Copie, C. Liu, M. E. Tillman, E. D. Mun, J. Schmalian, S. L. Bud'ko, M. A. Tanatar, P. C. Canfield and A. Kaminski "Momentum dependence of the superconducting gap in NdFeAsO<sub>0.9</sub>F<sub>0.1</sub> single crystals measured by angle resolved photoemission spectroscopy" Physical Review Letters, 2008, 101, 147003. DOI 10.1103/PhysRevLett.101.147003 Cited 166 times.

A. I. Goldman, D. N. Argyriou, B. Ouladdiaf, T. Chatterji, A. Kreyssig, S. Nandi, N. Ni, S. L. Bud'ko, P. C. Canfield and R. J. McQueeney "Lattice and magnetic instabilities in CaFe<sub>2</sub>As<sub>2</sub>: A single-crystal neutron diffraction study" Physical Review B, 2008, 78, 100506. DOI 10.1103/PhysRevB.78.100506 Cited 164 times.

Mazin, I.I. and J. Schmalian "Pairing symmetry and pairing state in ferropnictides: Theoretical overview" Physica C-Superconductivity and Its Applications, 2009, 469, 614-627. DOI 10.1016/j.physc.2009.03.019 Cited 159 times.

J. A. Anderson, C. D. Lorenz and A. Travasset "General purpose molecular dynamics simulations fully implemented on graphics processing units" Journal of Computational Physics, 2008, 227, 5342-5359. DOI 10.1016/j.jcp.2008.01.047 Cited 158 times.

#### ○ Cover Articles

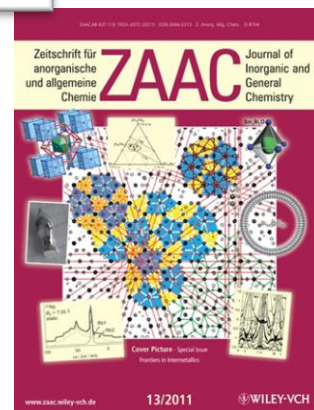
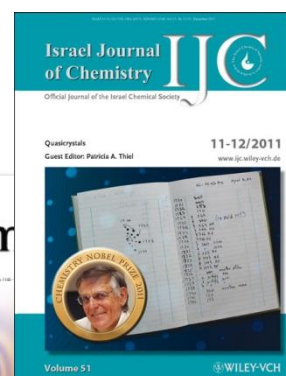
P. A. Thiel "Guest Editorial: Quasicrystals" Israel Journal of Chemistry, 2011, 51, 1141-1142. DOI 10.1002/ijch.201100127.

X. K. Fang, P. Kogerler, M. Speldrich, H. Schilder and M. Luban "A polyoxometalate-based single-molecule magnet with an S=21/2 ground state" Chemical Communications, 2012, 48, 1218-1220. DOI 10.1039/c1cc15520b.

S. Thimmaiah, N. A. Crumpton and G. J. Miller "Crystal Structures and Stabilities of gamma-and. gamma '-Brass Phases in Pd(2-x)Au(x)Zn(11) (x=0.2-0.8): Vacancies vs. Valence Electron Concentration" Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 1992-1999. DOI 10.1002/zaac.201100357.

#### ○ Journal Articles Published in FY2012 in Journals with Impact Factors > 10

T. P. A. Ruberu, H. R. Albright, B. Callis, B. Ward, J. Cisneros, H. J. Fan and J. Vela "Molecular Control of the Nanoscale: Effect of Phosphine-Chalcogenide Reactivity on CdS-CdSe Nanocrystal Composition and Morphology" ACS Nano, 2012, 6, 5348-5359. DOI 10.1021/nn301182h



E. M. Levin, S. L. Bud'ko and K. Schmidt-Rohr "Enhancement of Thermopower of TAGS-85 High-Performance Thermoelectric Material by Doping with the Rare Earth Dy" *Advanced Functional Materials*, 2012, 22, 2766-2774. DOI 10.1002/adfm.201103049

M. Cai, Z. Ye, T. Xiao, R. Liu, Y. Chen, R. W. Mayer, R. Biswas, K. M. Ho, R. Shinar and J. Shinar "Extremely Efficient Indium-Tin-Oxide-Free Green Phosphorescent Organic Light-Emitting Diodes" *Advanced Materials*, 2012, 24, 4337-4342. DOI 10.1002/adma.201202035

L. H. Xiao, L. Wei, C. Liu, Y. He and E. S. Yeung "Unsynchronized Translational and Rotational Diffusion of Nanocargo on a Living Cell Membrane" *Angewandte Chemie-International Edition*, 2012, 51, 4181-4184. DOI 10.1002/anie.201108647

M. S. Gordon, D. G. Fedorov, S. R. Pruitt and L. V. Slipchenko "Fragmentation Methods: A Route to Accurate Calculations on Large Systems" *Chemical Reviews*, 2012, 112, 632-672. DOI 10.1021/cr200093j

T. van der Sar, Z. H. Wang, M. S. Blok, H. Bernien, T. H. Taminiau, D. M. Toyli, D. A. Lidar, D. D. Awschalom, R. Hanson and V. V. Dobrovitski "Decoherence-protected quantum gates for a hybrid solid-state spin register" *Nature*, 2012, 484, 82-86. DOI 10.1038/nature10900

J. Shinar "Organic Electronics: Organic thin-film magnetometers" *Nature Materials*, 2012, 11, 663-664. DOI 10.1038/nmat3390

P. Tassin, T. Koschny, M. Kafesaki and C. M. Soukoulis "A comparison of graphene, superconductors and metals as conductors for metamaterials and plasmonics" *Nature Photonics*, 2012, 6, 259-264. DOI 10.1038/nphoton.2012.27

R. Prozorov and V. G. Kogan "London penetration depth in iron-based superconductors" *Reports on Progress in Physics*, 2011, 74, 124505. DOI 10.1088/0034-4885/74/12/124505

K. Hashimoto, K. Cho, T. Shibauchi, S. Kasahara, Y. Mizukami, R. Katsumata, Y. Tsuruhara, T. Terashima, H. Ikeda, M. A. Tanatar, H. Kitano, N. Salovich, R. W. Giannetta, P. Walmsley, A. Carrington, R. Prozorov and Y. Matsuda "A Sharp Peak of the Zero-Temperature Penetration Depth at Optimal Composition in BaFe<sub>2</sub>(As<sub>1-x</sub>P<sub>x</sub>)<sub>2</sub>" *Science*, 2012, 336, 1554-1557. DOI 10.1126/science.1219821

C. T. Lefevre, N. Menguy, F. Abreu, U. Lins, P. Mihaly, T. Prozorov, D. Pignol, R. B. Frankel and D. A. Bazylinski "A Cultured Greigite-Producing Magnetotactic Bacterium in a Novel Group of Sulfate-Reducing Bacteria" *Science*, 2011, 334, 1720-1723. DOI 10.1126/Science.1212596

A. Travesset "Self-Assembly Enters the Design Era" *Science*, 2011, 334, 183-184. DOI 10.1126/science.1213070

Teck L. Tan, Lin-Lin Wang, Duane D. Johnson, and Kewu Bai, "A Comprehensive Search for Stable Pt–Pd Nanoalloy Configurations and Their Use as Tunable Catalysts," *Nano Letters* 2012 12 (9), 4875-4880. DOI 10.1021/nl302405k

**Invited Talks:**

- Total: 137
- 93 domestic
- 44 international

**Patents:**

- Iver Anderson and the late Bob Terpstra were awarded patent no. 8,197,574 on "Dispersoid Reinforced Alloy Powder and Method of Making."

**Awards:**

| Program | Recipient   | Award  |
|---------|---|--|
| AMCS    | Michelle Duncalf  | ISU LAS Award for Outstanding New Professional   |
| CBS     | Aaron Sadow   | National Academy Distinguished Young Scientist   |
| CBS     | Cynthia Jenks   | Elected AAAS Fellow  |
| CBS     | Javier Vela   | Made Hispanic Engineering magazine's "40 under 40" list of top young scientists and engineers.                         |
| CBS     | Robert S. Houk  | American Chemical Society Division of Analytical Chemistry Award in Spectrochemical Analysis                           |
| DMSE    | Danny Shechtman   | <b>2011 Nobel Prize in Chemistry</b>   |
| DMSE    | David Jiles   | Honorary Fellow of the Indian Society for Non-Destructive Testing  |
| DMSE    | Mei Hong  | Irving Sigal Young Investigator Award  |
| DMSE    | Michael Kessler   | 2011 ISU Award for Early Achievement in Research   |
| DMSE    | Min Gyu Kim   | 2012 Zaffarano Prize for Graduate Student Research   |
| DMSE    | Pat Thiel   | Fellow of the MRS  |
| DMSE    | Balaji Narasimhan   | Elected AAAS Fellow  |
| DMSE    | Sergey Bud'ko   | 2012 ISU P&S Research Award  |
| DMSE    | Paul Canfield   | <b>DOE Ernest Orlando Lawrence Award</b>   |
| DMSE    | Ruslan Prozorov   | American Physical Society Outstanding Referee<br>APS Fellow  |
| DMSE    | Ryan Goetsh   | ISU 2012 Student Employee of the Year<br>ISU Dept of Physics and Astronomy Mal Iles Innovation Award                   |
| DMSE    | Tanya Prozorov  | DOE Office of Science Early Career Research Award  |
| DMSE    | Vik Dalal   | Elected AAAS Fellow<br>2012 IBM Faculty Award  |
| DMSE    | John Clem   | 2012 IEEE Council on Superconductivity Award for Significant and Sustained Contributions for Applied Superconductivity |
| DMSE    | Alexander Spicher,<br>John Meyer,<br>Iver Anderson,<br>Joel Rieken,<br>David Byrd | Outstanding Poster Award from the 2012 International Conference on Powder Metallurgy & Particulate Materials           |
| ESH&A   | Ames Laboratory   | 2011 Bronze Incident Rate Award  |
| SMDS    | Gene Takle  | Fellow of the American Meteorological Society  |

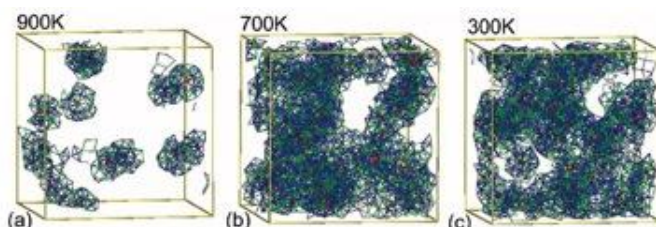


| Program | Recipient                    | Award   |
|---------|------------------------------|---|
| SMDS    | Mark Bryden<br>Doug McCorkle | 2012 FLC Midcontinent Excellence in Technology Transfer Award |
| SMDS    | Erin MacDonald               | ASME Design Automation Young Investigator Award               |

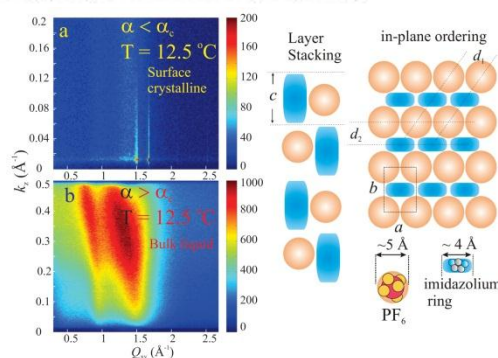
## Scientific Program Highlights (by Laboratory Program)

### Division of Materials Sciences and Engineering (DMSE)

- DMSE was successful in competing for ARPA-E REACT solicitation receiving two awards to address rare earth materials in permanent magnet materials. The first project led by the Ames Laboratory explores the possibilities of discovering a cerium based permanent magnet. While this is not a rare earth free material it does take advantage of the fact that there are abundant quantities of cerium as a result of the high demand for neodymium. In the second project, Ames Laboratory scientists will team with Pacific Northwest National Laboratory on research to reduce the cost of wind turbines and electric vehicles by developing a new alternative to rare earth permanent magnets based on an innovative composite that uses manganese materials
- In November 2011 Ames hosted an on-site BES Triennial review of 7 of its 14 ongoing BES-MSED funded FWP research projects. The on-site review was well received by both BES and peer reviewers who commented positively on how well the review was organized and the overall logistics of the 1½ day review. The outcome of the review was that all 7 FWP had compelling scientific directions with goals and objective aligned with both BES and Ames Laboratory missions. One FWP was awarded an increase in base funding while the other 6 FWPs were continued at current funding levels.
- DMSE produced 200 publications YTD; 12% of these publications appearing in high impact journals and submitted to BES-MSED as research highlights. These highlights are posted on the Ames Laboratory website.
- DMSE developed a new method for examining and describing atomic arrangements in disordered systems termed "order mining." Rather than focusing on the fine atomic details of the structure, the new method focuses on identifying larger motifs and determining patterns amongst these motifs. This method provides a powerful tool for quantifying changes in the chaotic arrangements of atoms as a liquid metal cools.
- An ordered "crystalline" phase was discovered on the surface of an ionic liquid at temperatures well above the melting point. These quasi-two-dimensional crystals consist of nanodomains which result from the reorientation of negative ions as they interact with molecules at the vapor-liquid interface.
- Genetic modification of the plant cellulose structure has been demonstrated for the first time. This discovery opens the opportunity to genetically modify the cellulose structure that is most compatible for sugar production.



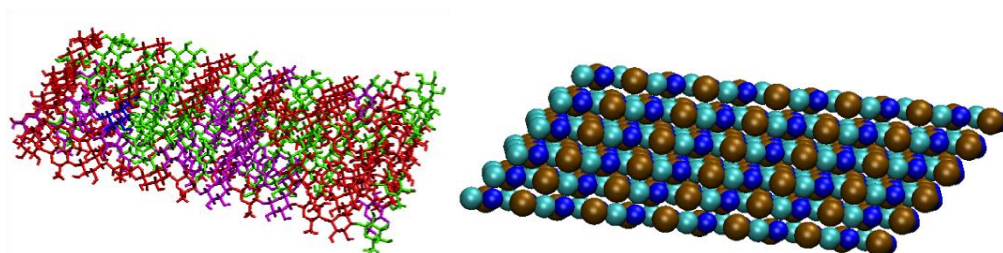
Development of ordered clusters as temperature is decreased in a glassy copper (green) and zirconium (blue) alloy.



- Development of a predictive tool for the selection of materials with optimum optical properties for use in metamaterials. The conducting materials used to make metamaterials are central to their efficiency and the potential impact of identifying appropriate materials could be huge, because of the considerable efficiency improvements that are possible.

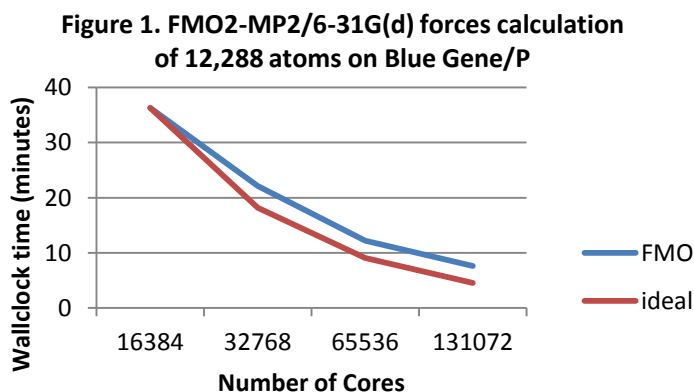
### **Applied Mathematics and Computational Sciences (AMCS) Program**

- Proposed and implemented a strategy to determine and pin shared data to specific memory banks in multicore nonuniform memory access (NUMA) architectures.
- Implementations of the all-to-all collective operations were studied as to their energy saving potential on a per call basis. The experiments, performed on the OSU MPI benchmarks and on a real-world CPMD code showed that the energy consumption was reduced by 10% to 15.7% with little performance degradation.
- Quantum and multi-site coarse grained molecular dynamics simulations were carried out for the cellulose I $\alpha$  microfibril. Quantum effects are needed to accurately predict the strength of binding interactions. Newly developed coarse-grained models effectively capture the residue scale motions, and hence enable simulation of long-time dynamics in cellulosic materials.

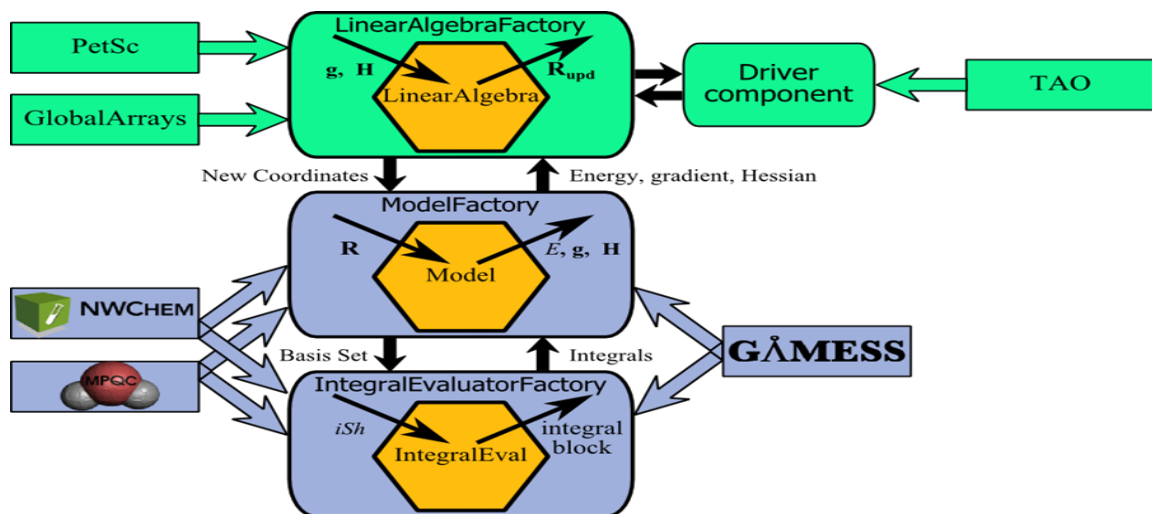


**Picture of a slice of cellulose**

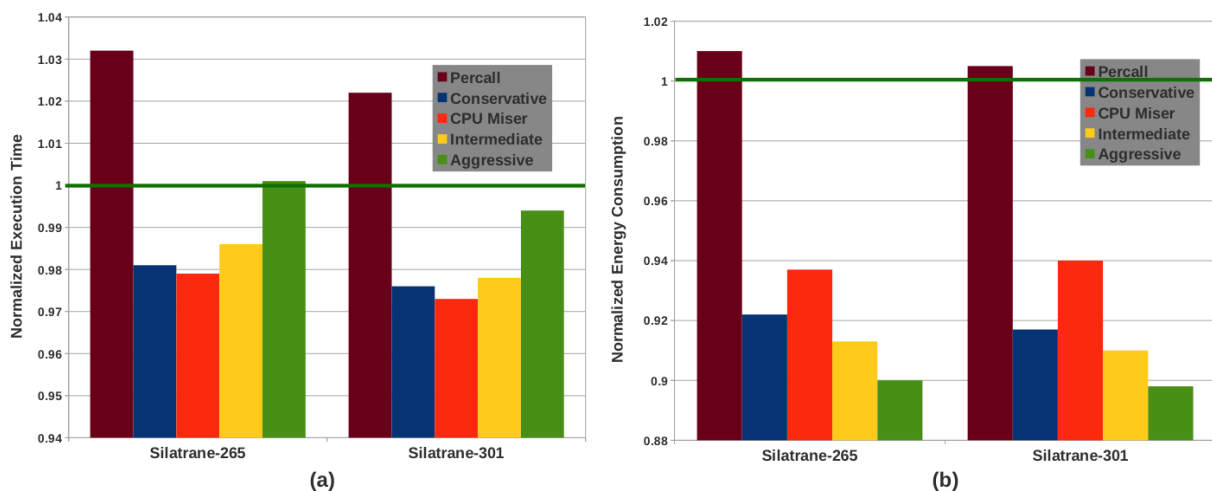
- Established, with the aid of an INCITE grant, that the fragment molecular orbital method in GAMESS scales almost linearly to 131,000 cores, thereby achieving petascale computing.



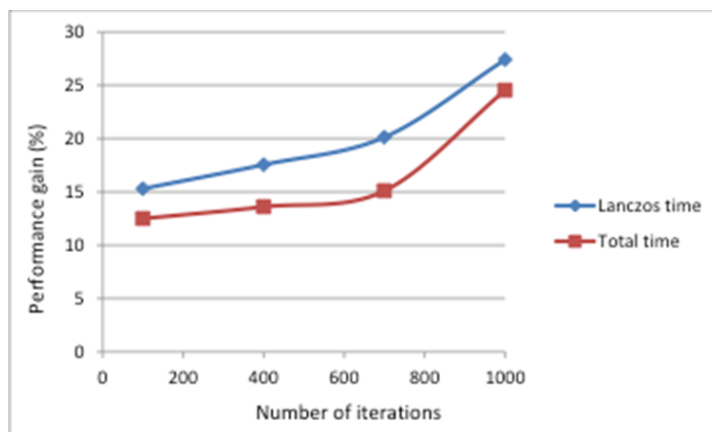
- As part of a SciDAC-E grant, the Princeton TigerCI code has been implemented successfully into GAMESS. In collaboration with Prof. Shirley Moore (University of Tennessee, Knoxville) and the TAU development group (University of Oregon), the TigerCI code was instrumented using the TAU performance analysis tool, and the major serial performance bottlenecks were identified and analyzed. The current efforts are concentrated on parallelization of the remaining major bottleneck.
- As part of the Common Component Architecture (CCA) SciDAC grant, we have implemented and tested the ability to make certain features of GAMESS available to other non-commercial codes. This has been reported in a paper that has been submitted to the Journal of Computational and Theoretical Chemistry (See figure below).



- Proposed and implemented a runtime procedure for the analysis of point to point communication calls and the in-between time gaps as to their potential for saving energy with dynamic voltage and frequency scaling of the processor. The experiments with the GAMESS package show close to the maximum (11%) energy savings with a low performance loss of 2% on the computing platform used, which compares favorable with existing state-of-the-art techniques. (See figure below)



- Proposed and implemented a strategy to determine and pin shared data, representing sparse of dense matrices, to specific memory banks in multicore nonuniform memory access (NUMA) architectures. Experiments with a realistic large-scale application revealed speedups of up to 25% as compared with the default memory placement policy. (See figure below)



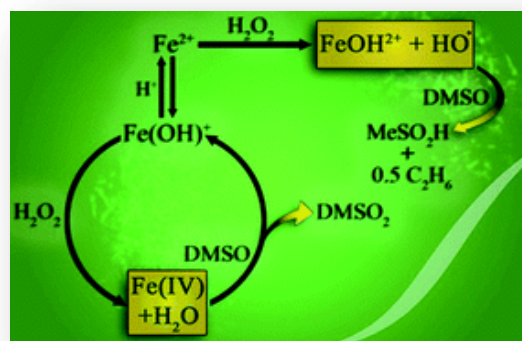
## Division of Chemical and Biological Sciences

### BES Program Reviews

- In the first quarter of FY2012, the triennial reviews for the FWP's within the Separation & Analysis and Energy Biosciences Programs of CSGB were held onsite. The review outcomes for both were positive. One FWP has been recommended for an increase in funding starting in FY2013.

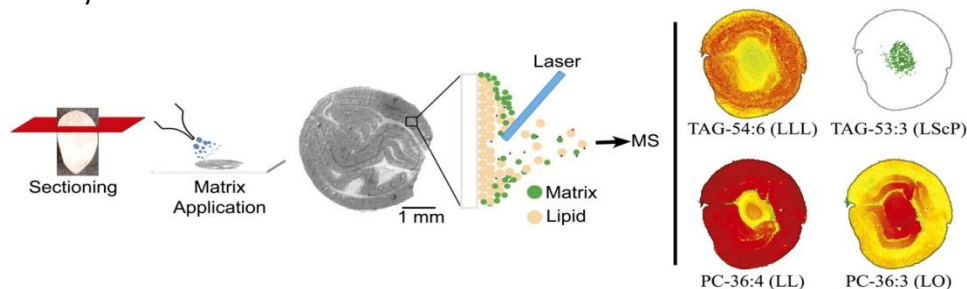
### BES Highlights

- Published 51 papers in FY2012 (as of 9/24/2012 according to ISI Web of Science).
- 22% of the papers published in FY2012 so far were in high impact journals (impact factor > 6).
- Dr. Brinkman and Dr. Kung included Ames Laboratory catalysis research in their slide presentations to BERAC and BESAC, respectively.
- BES/CSGB provided the funding necessary to replace a solid-state NMR console that was failing. This equipment is used 24/7 to support two BES projects. Additional funding was provided for a new mass spectrometer critical for success in our research on plant metabolites.
- Uncovered the exact nature of the intermediate in the widely used Fenton reaction. The Fenton reaction is used worldwide commercially to treat wastewater and also occurs in nature. This discovery explains the differences in products formed under certain reaction conditions and clears up an 80 year old debate.
- Designed advanced methods to make maps of the locations of molecules within plant materials. Many molecules are analyzed at once using a modified version of a very sensitive mass spectrometer in this



Fenton reaction pathways

technique known as matrix-assisted laser desorption/ionization-mass spectrometry imaging (MALDI-MS). Within cottonseed embryos, which are about 3/16<sup>th</sup> of an inch in diameter, this method (with 10 micron resolution) showed a surprisingly non-uniform mixture of lipids whose concentration varies with tissue functionality.



- Developed a novel design for ultraflat and ultrathin glass/polydimethylsiloxane (PDMS) hybrid microdevices to provide almost uncompromised optical imaging quality for on-chip super-localization and super-resolution imaging of single molecules and nanoparticles under a variety of microscopy modes. Super-localization of single molecules and nanoparticles with a precision of sub-nanometer to a few tens of nanometers is crucial for elucidating nanoscale structures and movements in biological and chemical systems.
- Established a new theory that shows that reactivity at catalytic sites inside narrow pores is controlled by how molecules move at the pore openings. The reaction behavior is similar to a busy grocery store, where customers roam multiple aisles, grabbing items off the shelves. Since the aisles get pretty full of customers throughout, most of the action will occur near the ends of the aisles, where shoppers can get in easily, grab items, and leave easily. Shoppers in the middle of the aisles will have a harder time passing each other and getting out of the aisle with their items. In the same way, the chemical reactions deep within the pores are limited. Until now it has been impossible to reconcile analytical theories with the findings of detailed step-by-step simulations. The new theory enables calculations of reactant and product distributions in minutes compared to the hours or days it takes to do the detailed simulations and yields comparable results. Thus, this new theory is a powerful tool for analyzing the catalytic behavior in these systems.
- Demonstrated, via an INCITE grant at Argonne National Laboratory, that high-level *ab initio* calculations can scale nearly linearly to more than 100,000 cores on a Blue Gene/P computer. Calculations using the fragment molecular orbital (FMO) method on more than 1,000 water molecules, at the second order perturbation level of theory, required less than 7 minutes for an energy + gradient run. It is anticipated that even more efficient calculations will become feasible once the FMO energy and gradient code are implemented on graphical processing unit architecture.

### BER Highlights

- Published 2 papers in FY2012 (as of 9/24/2012 according to ISI Web of Science).
- Attacked a significant problem for further development of IMAGETags. The problem is related to the nature of the ligand. The ligand needs to be able to readily penetrate the cell and also should not bind tightly to any cellular component. As a first step in this direction, we took a combinatorial approach in conjunction our SFA co-workers at LBNL to develop a ligand that has low retention in the cells. This ligand will be used to develop an aptamer that will then be incorporated into IMAGETags.
- Took delivery on robotic equipment, generously supported by BER, to dramatically speed up the development of new aptamers.

## **Education Programs**

- The Ames Laboratory set a new record for placing students/teachers and faculty in three distinct education programs for summer 2012. Those programs included the Science Undergraduate Laboratory Internship program (SULI), Community College Institute (CCI), and the Visiting Faculty Program (VFP). These programs involved 38 students and faculty from colleges and universities around the country.
- The Ames Laboratory Education Programs will begin offering a spring semester version of the Science Undergraduate Laboratory Internships (SULI) in spring 2013. The inaugural program will host three students for 16 weeks at the Laboratory. Students will work with the Lab scientists/mentors to do cutting-edge research.
- Education Programs participate in the Strengthening the Professoriate at ISU (SP&ISU) hosted Broader Impact Resource Fair held at ISU on April 4, 2012. The Laboratory joined with 25 other programs and partners involved in broader impacts, who met with faculty at ISU who would like to learn more about how to be involved in the Lab's programs.
- Forty teams of high school students and 16 teams of middle school students participated in the Ames Laboratory's High School and Middle School Science Bowls in January and February 2012, respectively. Approximately 100 scientists, staff and students volunteered for the High School Science Bowl. Approximately 60 scientists, staff and students volunteered for the Middle School Science Bowl. The Lab's Science Bowl coordinator participated on the media team for the National Science Bowl, which was held in Washington, D.C. in April/May 2012. The Laboratory's Director served as a moderator/judge for the competition.
- Science Undergraduate Laboratory Internship (SULI) students Jillian Gerkey and Daniel Murphy say their paper, "Structural and functional analysis of transcriptional regulator RV3066 of *Mycobacterium tuberculosis*" published in the 2012 issue of *Nucleic Acids Research*.
- Former Visiting Faculty Program (VFP) students Brandon Callis, Brittney Ward, Joana Cisneros and faculty member, Haujun Fan, saw their paper, "Molecular Control of the Nanoscale: Effect of Phosphine Chalcogenide Reactivity on CdS-CdSe Nanocrystal Composition and Morphology," submitted for publication in the March 2012 edition of the *Journal of the American Chemical Society*.

## **Midwest Forensics Resource Center (MFRC) (includes WFO federal partners)**

- The National Institute of Justice funded a research project to apply face recognition technology to microstamped cartridge cases to determine if microstamping is a viable technology to link a firearm to a cartridge. Research findings show that tools made successively on the same piece of equipment have enough individual characteristics in the tool markings that they can be separated 97% of the time.
- Research funded by the National Institute of Justice has developed a method of self-calibration of metal fracture matching that improves confidence of matching at multiple length scales. The result is a greatly improved understanding and confidence in this important type of forensic evidence, frequently encountered in criminal cases.
- With funding from DHS, we have assembled an ink and toner analysis database using surface analysis methods. The database will be used as a reference for forensic investigations carried out by the Homeland Security Investigations Forensic Laboratory of U.S. Immigration and Customs Enforcement.
- Ames Lab researchers have developed software algorithms to automatically substantially reduce the noise of the 3-D raw data from an optical profilometer and developed methods to rapidly re-sample the

raw data into regular grids at any given pixel size and any orientation with advanced computer graphics tools. These technologies were developed for application to forensic toolmark analysis, but also have application in other areas of surface analysis.

- An approach known as random probability match is being developed for the statistical comparison of mass spectral data obtained using gas chromatography-mass spectrometry to provide a statistical measure of the likelihood of incorrect identification of a compound. While method development is using mass spectra of controlled substances in forensic analyses, the procedure can be readily applied to mass spectral data for other types of chemical analyses.
- A novel physiological model is being designed and constructed to study the dynamics of firearms-related blood spatter. The model is suitable for simulation of cranial gunshot wounding and associated spatter formation.
- A wide range of analytical chemical methods are being applied to the problem of characterization of designer drugs to aid law enforcement in the identification of these rapidly evolving drugs of abuse.
- Researchers are investigating the 3D spatial frequency of a material's fracture surface to establish the underlying scientific basis for quantitative forensic analysis and differentiation of fractured and torn surfaces, by employing the fundamentals of fracture mechanics and the nature of the material behavior. This research, conducted in response to the NIJ's expressed need for knowledge underlying forensic science disciplines, and in collaboration with practicing forensic scientists, arose from the core Applied Materials Science and Engineering capabilities of the Ames Laboratory.
- Development of femto-second laser ablation – inductively coupled plasma – mass spectrometry for isotopic analysis of plant and other organic matrices has shown excellent sensitivity for rapid analyses with little or no sample preparation. This project has built on long term investments by DOE in materials characterization and analysis at the Laboratory.

Based upon the above information, the Laboratory assesses its progress in meeting Goal 1 as an A.



## Goal 3.0 Provide Effective and Efficient Science and Technology Program Management

### 3.1 Provide Effective and Efficient Strategic Planning and Stewardship of Scientific Capabilities and Program Vision

#### Highlights by Objective:

##### Scientific Planning

- The Ames Laboratory's current strategic plan was approved in October of 2011. Since then this plan has been used to develop the annual lab plan presented to DOE and guides our allocation of resources. The execution of the strategic plan enables a research portfolio that takes advantage of the Lab's unique capabilities and strengthens our core competencies in Condensed Matter Physics and Materials Science, Chemical and Molecular Science and Applied Materials Science and Engineering.
- In FY12, Laboratory Management developed a strategic plan for the Ames Laboratory Material's Preparation Center. This plan is under review by the Ames Laboratory Executive Council.
- The CRO implemented a yearly Laboratory-wide gathering entitled "Year in Review and Strategic Vision for the Future," not only to share information widely but to solicit input outside normal avenues.
- As part of our stewardship of our scientific capabilities and vision for the future, including signature materials discovery, design, and synthesis and processing efforts, we are focusing on the Sensitive Instrument Facility (SIF) and improved scientific computing facilities. A site for the SIF has been identified, and architectural plans as well as instrument inventory lists are being developed for the new facility. More details are in section 3.2
- Laboratory leadership will implement an LDRD program in accordance with DOE O 413.2B starting October 1, 2012. The LDRD Plan was submitted to DOE August 15, 2012 for approval. Funded projects will comply with the requirements set forth in the Laboratory's documented plan.
- With BES/MSED seed funding in 2010-2011, we have developed a highly coupled experimental and computational materials design/synthesis effort exemplified in ternary topological insulators. Critical intrinsic defects were predicted to control the reliability of topological insulator behavior, which has been confirmed experimentally, after single-crystals were synthesized in 2011/2012 and resistivity and Hall measurements were completed in August 2012.
- Based on part of our signature Materials Design and Synthesis efforts described above, we competed successfully for two ARPA-E REACT projects involving highly integrated experimental and computationally-driven design/synthesis of rare earths and permanent magnets for societal use; "*Novel High Energy Permanent Magnet without Critical Elements*" and led by AMES and "*Development of MnBi/Al Based Permanent Magnet with 40 MGOe at 200°C*" lead by PNNL.
- With the support of our Contractor, ISU, a new Materials Sciences and Engineering (MSE) course in Rare Earths was offered this Spring semester and taught by an Ames Laboratory scientist.
- Ames Laboratory strategically invested resources to acquire a HPC cluster (~14 Tflops) to support and enhance the "materials discovery, design and synthesis and processing" based initiative, using internal and mid-year DOE/BES equipment grants. More details are in section 3.2.
- Again, as part of our signature Materials Design efforts, and at ARPA-E's suggestion from a well-reviewed REACT proposal in 2011, we submitted in July to ARPA-E FCE open call a proposal entitled "*Solid State Processing of Fully Dense Anisotropic Nanocomposite Magnets*".
- The Ames Laboratory Division of Chemical and Biological Sciences continue to search for a strategic senior hire in the area of catalysis in collaboration with our Contractor as part of our catalysis initiative.



- The Laboratory held a joint international workshop with PNNL on solid-state NMR to discuss scientific drivers for future instrumentation and key advancement needs. This workshop was part of our implementation of our Center for Solid State NMR Science initiative.
- With funding from DHS, we have assembled an ink and toner analysis database using surface analysis methods. The database will be used as a reference for forensic investigations carried out by the Homeland Security Investigations Forensic Laboratory of U.S. Immigration and Customs Enforcement.
- We developed matrix-assisted laser desorption mass spectrometry—mass spectral imaging (MALDI-MSI) for chemical analysis (including separation of structural isomers) of plants with excellent sensitivity and 10 micron resolution.
- Our development of femto-second laser ablation – inductively coupled plasma – mass spectrometry for isotopic analysis of vegetation and other organic matrices has shown excellent sensitivity for rapid analyses with little or no sample preparation. This project has built on long term investments by DOE in materials characterization and analysis at the Laboratory.
- We are developing the Random Probability Match approach for statistical comparison of mass spectral data obtained via gas chromatography-mass spectrometry to provide a statistical measure of the likelihood of incorrect compound identification, relevant to many fields including forensics.
- We developed new software algorithms to provide automated substantially reduced noise in 3-D raw data from an optical profilometer and developed methods to rapidly re-sample the raw data into regular grids at any given pixel size and any orientation with advanced computer graphics tools. These technologies were developed for application to forensic toolmark analysis, but also have application in other areas of surface analysis.

#### Scientific and Technology Staffing

- The Ames Laboratory Division of Chemical and Biological Sciences continues discussions with several external researchers as part of our search for a strategic senior hire to provide leadership in catalysis and support our catalysis initiative. This potential hire is being coordinated with ISU and the ISU Department of Chemistry. Regular updates are provided to BES/CSGB.
- The Ames Laboratory Division of Materials Science and Engineering has made an offer and is negotiating with a potential mid-career hire in rare-earth metallurgy to support our Center for Rare-Earth and Energy-critical Materials (CREEM) initiative. This is a cooperative search utilizing resources at Ames Laboratory, ISU and the ISU Department of Materials Science and Engineering.
- We have hired 12 researchers to support new funding from ARPA-E and Fusion Energy.

Based upon the above information, the Laboratory assesses its Strategic Planning and Stewardship of its Scientific Capabilities and Vision as an A.

#### 3.2 Provide Effective and Efficient Science and Technology Project/Program/Facilities Management

- In November 2011 Ames hosted an on-site BES Triennial review of 7 of its 14 ongoing BES-MSED funded FWP research projects. The on-site review was well received by both BES and peer reviewers who commented positively on how on well the review was organized and the overall logistics of the 1½ day review. The outcome of the review was that all 7 FWP had compelling scientific directions with goals and objective aligned with both BES and Ames Laboratory missions. One FWP was awarded an increase in base funding while the other 6 FWPs were continued at current funding levels.  
 “Overall, the reviewers commented that the BES-supported projects have produced strong scientific results in topical areas that are relevant to the BES mission and well-aligned with the core competencies of Ames Laboratory.”

- The DMSE Program Management realigned efforts of two FWP's to strengthen and enhance both, in consultation with BES/MSED. This realignment was successfully reviewed during the BES/MSED triennial review discussed above.
- The Laboratory continued progress on the Sensitive Instrument Facility, identified in the 2011 Lab Plan as one of our critical facilities needs to support Laboratory missions and programs. Since then, funding totaling \$5.5M has been received from the Office of Science for the project. The Site Evaluation Study by outside consultants has been completed. The procurement of A/E design services is complete and a first deliverable, the Program Report, was received. Work continues on the next set of deliverables.
- DMSE awaits delivery of two key computer clusters to support our signature efforts in Materials Design and Design of Metamaterials, capitalizing on our theoretical and computational advances. For materials design, with half of the cost from DOE mid-year equipment request, we have ordered a \$972K HPC cluster based on low-energy Intel chips for lower operational costs, having 164 dual-processor nodes (1968 cores), large RAM/core and very fast (56 GB/s) infiniband communications between nodes, and with solid-state (240 GB) drives for rapid data-transfer to each core. The second computer, for design of anisotropic metamaterials and plasmonic nanostructures, is a smaller 8-node cluster with very large (128 Gb/node) memory for time-domain and finite-element modeling.
- DMSE continues to expand & develop fabrication and characterization capabilities that enable testing of theory/modeling over a broad spectrum of materials.
- Two AMES BES/CSGB FWP's were reviewed onsite in December. This successful triennial review resulted in the recommendation of one FWP for increased funding in FY2013 and a potential for increased funding of another. The successful review of both programs represents a successful transition in leadership following the retirement of a preeminent researcher.
- The AMES Division Director of Chemical and Biological Sciences held an internal white paper competition for new research ideas to enhance our Chemical and Molecular Sciences core competency and make progress on our catalysis initiative. 14 white papers were received. Two were selected by Laboratory management to be discussed with DOE Program Managers. Based on those discussions, one has been selected to provide a full proposal for a BES call and the other will be submitted as a white paper to BES/CSGB at their request.
- CBS implemented an annual call for prioritized equipment needs for all BES/CSGB FWP. The Division Director for Chemical and Biological Sciences developed a yearly budget and contingency plans to ensure program robustness against scientific and fiscal conditions. Tough staffing decisions were made in FY2012 resulting from poor research progress and fiscal concerns.
- The Mission Readiness team held their annual formal planning and review meetings with Laboratory Management, Department Managers and Scientific Program Directors to evaluate the mission readiness of facilities and infrastructure. The Mission Readiness team includes the Assistant Director for Scientific Planning, the Chief Operations Officer and the Manager of Facilities Services. These meetings provide valuable input for the planning process that is used in the preparation of the Annual Lab Plan.
- The Laboratory continues to make progress on the Sensitive Instrument Facility. The 2011 Lab Plan identified this as one of the critical facilities and infrastructure projects needed to support Laboratory missions and programs. Since then, funding totaling \$5.5M has been received from the Office of Science for the project. The Site Evaluation Study has been completed by outside consultants and the procurement of A/E design services is in progress.
- The Spedding Auditorium renovation is completed. This facility provides state of the art conference and presentation space. The facility has extensive A/V, networking, and distance learning capability. It provides great flexibility to support different types of meetings and presents an excellent image of

the Laboratory to visitors and staff. It was used for the first time for the visit of Deputy Secretary of Energy Ponneman. The video conferencing capabilities were used by DMSE for its annual BES-MSED Management review.

- Emily Smith was asked by her Program Manager to be co-chair of the DOE SC BES Division of Chemical Sciences, Geoscience and Bioscience, Separations and Analysis PI meeting in April.
- Robert McQueeney became a detailee for the Scientific User Facility Neutron Instrumentation Program.

Based upon the above information, the Laboratory assesses its Technology Project/Program/Facilities Management as an A-.

### 3.3 Provide Efficient and Effective Communications and Responsiveness to Headquarters Needs

- HQ requests for information are provided before their requested due date or on time.
- The Director communicated his 100<sup>th</sup> biweekly Director's Message to all employees and associates, and continues the series, unbroken.
- The Director holds semi-annual town hall meetings with various constituencies of the Lab's personnel.
- Scientific managers have put in place regular communication plans with their counterparts in DOE. Scientific highlights and progress are communicated on a consistent basis. 36 highlights were submitted in FY2012.
- Scientific Division Directors hold regular meetings with their scientists.
- Scientific Division Directors regularly attend BESAC and BERAC meetings.
- The BES/CSGB laboratory coordinators meets regularly with BES/CSGB team leaders and program managers. A list of all papers resulting from funding are provided on a quarterly basis. Highlights of high impact papers are provided regularly.
- The CRO reports and consults with Program Managers in Germantown regularly regarding Ames Laboratory science programs, beyond the, e.g., Lab Management and other reviews.
- The Office of Sponsored Research Administration responded to the Foreign MOU datacall and also provided an MOU Plan for Foreign Entities to HQs as required. The MOU Plan was approved and is now implemented.

Based upon the above information, the Laboratory assesses its Effective Communications and Responsiveness to Headquarters as an A.

### Notable Outcome

#### 3A: (BES) Refine the strategic vision for, and continue execution of, a signature effort on materials discovery and design. (Objective 3.2)

- Materials Discovery and Design is a mission driven scientific initiative of the Ames Laboratory that rests on the Laboratory's underlying scientific cornerstones. It brings together and unites several related efforts that become mutually supporting, enabling the Laboratory to perform at a higher level in this area, as demonstrated by its success in competing for new funding.



#### Progress to Date:

- Via 2010-2011 seed funding (BES), we have developed and published results from our highly coupled experimental and computational materials design/synthesis effort exemplified in ternary topological insulators.
- From our signature materials discovery and design efforts, we competed successfully and initiated two ARPA-E REACT projects involving highly integrated experimental and computationally-driven design/synthesis of rare earths and permanent magnets for societal use; *"Novel High Energy Permanent Magnet without Critical Elements"* led by AMES and *"Development of MnBi/Al Based Permanent Magnet with 40 MGOe at 200°C"* lead by PNNL.
- As a result of our signature discovery and design efforts for the REACT Program, and at ARPA-E's suggestion, we submitted to ARPA-E FCE call the proposal *"Solid State Processing of Fully Dense Anisotropic Nanocomposite Magnets"*.
- The Ames Laboratory DMSE awaits delivery of a HPC (56 Gb/s Infiniband) cluster to support and enhance the "materials discovery, design and synthesis and processing" initiative, using internal and mid-year DOE equipment grants (BES).
- For computational design and understanding of real anisotropic metamaterials and plasmonic nanostructures a large-memory compute cluster (8 Gb/core, 128 Gb/node) is being acquired from a mid-year DOE equipment grant (BES).
- We have completed installation of a high-P/high-T Gradient Bridgman Crystal Growth furnace to grow single crystals of intermetallics and oxides containing highly chemically reactive constituents and/or high vapor pressures, or compounds with near congruent melting (BES).
- The acquisition and assembly of an inert Atmosphere Glove box system for the synthetic discovery of new materials containing air reactive components is ongoing (BES).
- With the support of our Contractor, ISU, a new Materials Sciences and Engineering (MSE) course in Rare Earths was offered this Spring semester and taught by an Ames Laboratory scientist.
- Funding for a new computer cluster for designing non-RE based permanent magnets has been awarded (EERE-VT).
- The 2012 Lab Plan built upon our four Cornerstones for the strategic growth of the Laboratory. The Laboratory proposed two new initiatives in addition to three that were presented in FY2011:
  - ABACUS, i.e., Advanced Bit-manipulations, Algorithm & Code development for US, to develop algorithms needed for materials discovery. Progress to Date:
    - 3 full proposals were submitted to BES "Predictive Theory and Modeling" call involving Materials Genome Initiative.
    - AMES and ANL held planning meetings for joint Materials Genome algorithm efforts.
  - Center for Solid-State Nuclear Magnetic Resonance (SS-NMR) Science. Progress to Date:
    - Joint AMES/PNNL International Solid-State NMR Workshop (Dec 2011) about scientific drivers and key advancements needed.
    - First demonstration of the dramatic enhancement in signal-to-noise possible for catalytic materials using dynamic nuclear polarization NMR by AMES/Lille/Lausanne.
- To enhance SS-NMR capabilities, and impact signature Materials Discovery and Design/Characterization efforts, the Ames Laboratory and PNNL held jointly held an international conference on "Challenges for Advanced Nuclear Magnetic Resonance" 7-9 December 2011. The purpose was to assess new directions and the potential for high-resolution Dynamic-Nuclear-Polarization NMR to provide unparalleled resolution of chemical reactions. First data from Ames' DNP-NMR experiments in summer of 2012 showed a remarkable increase in resolution for catalytic reactions (publications in preparation)

Notable Outcome 3A was met. The Laboratory's overall assessment for meeting the objectives of Goal 3 is an A.

## Goal 4.0 Provide Sound and Competent Leadership and Stewardship of the Laboratory

### Highlights by Objective:

#### 4.1 Leadership and Stewardship of the Laboratory

- Laboratory leadership defined and refined the vision and strategic plan for research mission.
- The 2012 Lab Plan - the Plan built on the success of 2011's Plan and sharpened the focus on the Laboratory and DOE's strategic plans. The Plan provided progress-to-date for the 2011 Initiatives and was well received by DOE.
- Leadership developed an LDRD Plan in accordance with DOE O 413.2B and submitted it to DOE in August, 2012. Upon obtaining HQ approval, the CRO will implement the LDRD process starting October 1, 2012. Funded projects will comply with the requirements set forth in the Lab's documented LDRD Plan and Resource Request plan.
- Efforts in rare earth research are accelerating. The Laboratory has received more funding for DOE sponsored research and the number of contacts from non-DOE entities interested in rare earths grew significantly in FY2012.
- The Ames Laboratory developed several new strategic partnerships with leading U.S. industries in the critical rare-earth recycling and re-use arenas, including Advanced Recovery, Cytec Industries, GE Global Research, Molycorp, OLI Systems, Inc., Simbol Materials, as well as three National Laboratories with separations and advanced manufacturing facilities – INL, ORNL, and LLNL. From this one-and-half-year activity, the Ames Laboratory led a proposal submitted in August to EERE for a Critical Materials Hub.
- The Laboratory also developed relationships with other research groups in topics unrelated to the Critical Materials Hub but related to materials research in general.
- The Laboratory spun off a powder metallurgy company, Iowa Powder Atomization Technologies (IPAT) that received a DOE national award (the America's Next Top Energy Innovator award) for its potential impact on the US economy. This activity enhances the value of the Laboratory as seen by local communities and the state. The company is currently in negotiation for a license to the technologies as per their ANTEI option agreement.
- An Americas Next Top Energy Innovator optionee (IPAT) won the DOE's ANTEI challenge for titanium powder atomization. IPAT was also awarded first prize in the 2012 John Pappajohn Iowa Business Plan Competition, announced September 27, 2012.
- Laboratory scientists have continued to build relationships with vendors to serve as beta sites for new equipment. This gives our scientists a competitive advantage by gaining access to new scientific capabilities before the general scientific community.
- The Laboratory hosted a celebration of the accomplishments of Nobel Prize winner Danny Shechtman. Many of the members of ISU and Laboratory leadership and DOE-Chicago were present including new ISU President Steven Leath, as well as the Ames Site Office Manager, Cynthia Baebler.
- Deputy Director Harmon has stepped down from his leadership position, as of September 1, 2012, to focus on teaching and his research. An Interim Deputy Director will soon be named to serve until a national search is completed.
- The Laboratory stood up a proposal team to respond to the Critical Materials Hub proposal. This was an experiment to see if a more formally organized effort would help produce better proposals as part of a Proposal Review Committee recommendation. With the proposal now submitted the Director will work with those involved to evaluate the process.
- Laboratory leadership continues to work on its succession plan by working with Human Resources to identify gaps in departmental staffing and to determine the impact of loss in certain positions. The

Laboratory has approved strategic hiring in the Human Resources Office, the Budget Office and the Purchasing Office. ISU is engaged with the Laboratory in two strategic hires in the research areas.

- Scientific staff succession planning continues and negotiations are underway with a strong female candidate in rare-earth sciences.
- The Laboratory Director formed a Committee to review the recommendations that came out of the Proposal Review Committee report in late FY2011. The recommendations included improved spreadsheet models deployed to the research staff for building initial budgets, a better understanding for the review process and responsibilities and identified the need for an electronic routing and approval software package (See notable target 6B). Implementation of the committee's recommendations has been slowed by the preparation of a large Energy Innovation Hub proposal, which has also been used as a learning exercise, increasing the Lab's capacity to cope with large-scale efforts of this kind. Work continues on the proposal process, overall, but interim milestones include
- The Director created, on an experimental basis, a dedicated Proposal Team to guide and assist in the preparation of major proposals. The first project for this team was the Energy Innovation Hub proposal.

Based upon the above information, the Laboratory assesses its Leadership and Stewardship activities as an A-. This rating is based on Laboratory Management's focus on the Laboratory's research mission on Materials Discovery and Design and in managing the opportunities presented by all the interest in rare-earth elements.

#### 4.2 Management and Operation of the Laboratory

- Ames hosted its Contractor Assurance Peer Review in November, 2011 (See notable target below). The review team noted in the final summary paragraph of the peer review team's report:  
"The observations noted in this report indicate that the key elements of the CAS are in place and functioning as intended... In its present state, the Ames Lab CAS is delivering benefits and positive impacts, and has strengthened the foundations of the partnership among ISU, AMSO and Ames Lab."
- Ames Laboratory, ISU and the AMSO have determined which opportunities for improvement will provide the most cost-benefit and will focus on those two (Identify most pressing risks, and identify most useful metrics to use as key indicators).
- The Laboratory is providing quarterly institutional cost reports to DOE and will participate in the upcoming peer review process for the ICRs.
- The Laboratory COO is a member of the Office of Science Laboratory's Operations Improvement Council which is looking for opportunities to work together and leverage cost reduction actions from various locations. The group has set a series of goals to reduce operations costs.
- The Laboratory completed a project to improve our auditorium and conferencing space.
- The Laboratory implemented several new software packages over the past year:
  - CyberTrain: employee training management software.
  - OHM: occupational medicine patient tracking software.
  - eAppraisal: performance appraisal software .
  - Phone database: used to track telecommunication costs by project.
- eAppraisal has been presented to ISU HR staff as a best practice in the appraisal process and the Laboratory plans to share our experience with other Laboratories' HR officers as well.
- The Laboratory benefited from over \$300,000 savings on negotiated procurement actions.

- The Facilities and Engineering Services group has completed relining half of the fume hood stacks in Spedding Hall producing a sizable reduction in the amount of air moving through the stacks. We anticipate that this could reduce our heating costs by approximately 10%.
- Dr. King continues his “Director’s Message” on a bi-weekly basis. Many of these messages address current issues or expectations, accomplishments, opportunities, etc. This communication is shared with the Ames Site Office and other interested parties.
- The Director and Public Affairs have been working on a campaign to help scientists write articles based upon our scientific discoveries for the general public. articles in a way that the public can read and appreciate. This has helped to raise the awareness of the public as to the activities of Ames Laboratory. Three news releases have been written thus far in 2012 based on scientific highlights. These releases have resulted in over 60 media placements in outlets, such as R&D Magazine, Physics News and Science Daily. Combined, these releases have generated approximately 22K Google hits.
- Laboratory leadership continues to meet with DOE officials both locally and in Washington, D.C. In addition to on-site peer reviews, the Laboratory hosted DOE Deputy Secretary Ponemon in March and Office of Science COO McBrearty in July.
- Laboratory leadership worked with DOE-BES to justify additional funding for the Sensitive Instrument Facility. To date \$5.5M has been sent to the Laboratory to support the SIF. The programming and detailed design phase is underway.
- Sustainability efforts continue with work on the fume hood stacks, lighting changes, purchasing EPEAT and Energy Star devices, changing out UPSs, altering facility configurations and other small projects. We estimate that our efforts will reduce energy costs in excess of 10%.
- The Metals Development Building experienced a fire in the electrical switch gear. The Ames Fire Department extinguished the fire and the ISU Facilities Planning and Management staff helped the Laboratory get the building back on line the same day as the fire.

The Laboratory assesses its Management and Operations activities as an A-. This is based on the favorable outcome of the CAS peer review, the business system improvements, procurement savings and sustainability efforts.

#### 4.3 Contractor Value-added

- Ames Laboratory partnered with ISU and AMSO on the CAS Peer Review. ISU leadership present included President Geoffroy, Executive VP/Provost Hoffman, Executive VP for Business and Finance Madden, and VP for Research and Economic Development Quisenberry. Also participating were ISU’s members of the Operations Review Committee. The Peer Review team was impressed at the level of corporate involvement in Laboratory operations.
- ISU has committed to hire a new faculty position that will focus on rare earth research. This position will matrix into the Laboratory to work under Dr. Karl Gschneidner.
- ISU and the Lab continue to support joint-appointed faculty. Of the 47 faculty scientists with joint appointments 27 received 100% of their support from ISU for the academic year.
- ISU Facilities Planning and Management is working with Laboratory Management to plan for and locate the Sensitive Instrument Facility. Support has included meetings to discuss the construction process, the facility location, capacity of existing facilities, lease terms and the Regents approval process. Dean Morton also participated in the selection process for the professional services contract for the detailed design.
- ISU continues to provide half of the earned performance fee for the use of the Laboratory Director on related Laboratory business (\$157,450 in FY2012).



- ISU continues to provide half of the amount normally charged departments for tuition support for students assigned to Ames Laboratory (\$288K in FY2012).
- The ISU Vice Provost for Research has been working with Laboratory leadership in planning for the location of a new research facility that will be proposed this fall. Given the growth of the university this has developed into a difficult task but many options are being explored.
- Laboratory leadership has begun discussion with ISU on the possible options for the Laboratory to improve its computing facilities. The Laboratory will develop a formal list of needs and the Contractor will develop an inventory of available space.

The Laboratory assesses its Contractor-Value activities as an A-. This is based on ISU's efforts to help the Laboratory construct its Sensitive Instrument Facility and its efforts to mitigate the damages caused by the electrical fire in Metals Development.

## Notable Outcomes

### **4A: Host a Contractor Assurance System (CAS) Peer Review, prepare a written evaluation of the review team's opportunities for improvement, including a plan of action for those recommendations deemed beneficial to implement, and demonstrate senior-level leadership in and embracement of CAS implementation. (Objective 4.2)**

- Ames hosted its Contractor Assurance Peer Review in November, 2011. The team noted in the final summary paragraph of the peer review team's report:
  - “The observations noted in this report indicate that the key elements of the CAS are in place and functioning as intended.... In its present state, the Ames Lab CAS is delivering benefits and positive impacts, and has strengthened the foundations of the partnership among ISU, AMSO and Ames Lab.”
- ISU's Executive Vice-President for Business and Finance, the Ames Site Office Manager and the Ames Laboratory Director co-signed an evaluation of the CAS peer review Opportunities for Improvement and co-committed to the two action plans: developing a risk registry and developing high level metrics to help manage and evaluate the Laboratory. The document was finalized in September 2012. The co-signing of the document provides further evidence of the partnership that exists between the three institutions in regards to CAS and the Ames Laboratory.
- Two of the top risks identified by the partnership are succession planning and adequate facilities. In response to these concerns the Laboratory addressed both in its annual lab plan. DOE has placed a notable target in the 2013 PEMP goals regarding the development of a formal succession plan and has provided additional GPP funding for facility improvements and for the Sensitive Instrument Facility.
- CAS continues to be a topic of discussion between the Labs and DOE leadership as well as between members of the Executive Council, ISU, AMSO, and Laboratory managers and directors. This continued emphasis helps to continue the focus on CAS and on improving our CAS partnership.
- AMSO Manager is constantly looking for opportunities to reduce reviews or to partner with the Laboratory or ISU on reviews to reduce the time and frequency of reviews. This is possible because of the increased level of trust and the improved spirit of cooperation among the three partners.
- Develop an active and continuous succession plan to support growth and sustainability of the workforce. This will be accomplished by developing risk assessments and gap analysis by major areas within the Laboratory on a prioritized basis.
- Strengthen Leadership in MPC
  - Ongoing – Draft Strategic Planning document under Ames Laboratory management review

- Working with Iowa State University on potential faculty hires.
  - New rare earth hire underway (Corbett/Gschneidner)
  - Increase Depth in Solid State Theory (Schmalian)

Notable Outcome 4A was met.

The Laboratory's overall assessment for Goal 4 is an A-.

## Goal 5.0 Sustain Excellence and Enhance Effectiveness of Integrated Safety, Health, and Environmental Protection

### Highlights by Objective:

#### 5.1 Provide an Efficient Worker Health and Safety Program

- Ames Laboratory received a 2011 Bronze Incident Rate Award from the Iowa-Illinois Safety Council for an incident rate less than the national average for the applicable North American Industry Classification System (NAICS) code. The Ames Laboratory did not experience any recordable injuries or DART cases in FY2012, and recorded six first aid cases.
- In March 2012, the Ames Laboratory received a 2011 Bronze – GreenBuyAward reaching the Leadership Goal for three products in two different categories, and thereby achieving excellence in Sustainable Acquisition.
- In May 2012, the Ames Laboratory received a Certificate of Achievement for Excellence in Reporting to the Nuclear Materials Management and Safeguards System (NMMSS) for outstanding performance for inventory and reconciliation during 2011.
- Two ORPS reports were filed in 2012. One was related to suspect/counterfeit bolts found during the annual hoist and rigging inspection [SC—AMES-AMES-AMES-2012-0001- Suspect/Counterfeit and Defective items.]. Another was related to a fire in the electrical switchgear in the Metals Development Building on June 29, 2012 [SC—AMSO-AMES-AMES-2012-0002 – Switchgear Fire in Metals Development – Significance Category 3].
- The Spedding Hall HVAC, the access control, and the auditorium remodel projects are being conducted according to lessons learned regarding safety oversight and controls from previous HVAC upgrades and access control projects to assure protection of craft workers and building occupants.
- An NTS report was filed in 2012. The NTS was related to a nurse not renewing her license to practice [NTS—AMSO-AMES-AMES-2012-0001 – Lapse of Registered Nurse License].

The Laboratory assesses its worker health and safety activities as an A based on the Laboratory's receipt of 3 awards relating to ES&H, on having no recordable injuries or DART cases in FY2012 and its robust safety systems such as readiness review and the walk-through program and its overall safety culture.

#### 5.2 Provide Efficient and Effective Environmental Management System

- An Environmental Management System (EMS) Assessment was performed at Ames Laboratory, June 25-28, by a team from the DOE Chicago Office. The purpose was to conduct a formal assessment by a qualified party outside the control or scope of the EMS relative to specific requirements of DOE Order 436.1 (including the embedded ISO 14001:2004 requirements). Minor Nonconformities were identified in four elements and corrective actions have been initiated.
- The EMS is being re scoped to more clearly include the DOE sustainability goals. A new EMS Description will fully document the ISO requirements and sustainability elements.
- Fume hood discrepancies increased 113% (Jan-Aug 2012) when compared to the same period for 2011. The increase was a result of several power outages during June-August.
- The EMS Steering Committee (EMSSC) recommended two goals for CY2012. In February the EMSSC met with the Director and Chief Operations Officer to discuss the goals and other related topics.
- The Laboratory's EMS specialist, Dan Kayser, participated in an environmental management audit at PPPL and his knowledge, professionalism and ability to work as a team member were significant contributions to a successful audit.

- As a result of the Laboratory's Environmental Management System Assessment in June 2012, the Laboratory will formally include DOE's sustainability goals in an EMS Description document. This document will also address other corrective actions/opportunities for improvement which will help bolster the Environmental Management System.
- Additional projects that will reduce the Laboratory's impact to the environment include the exhaust stack lining project for Spedding Hall (over 50% stacks have been completed) and replacing inefficient light ballasts (~1100 light ballasts have been replaced since 2008).
- White paper usage was reduced by 28% (Jan-Aug 2012) as compared to the same period in 2011.

Based upon the above metrics, the Laboratory assesses its environmental management system activities as a B+.

The Laboratory's overall assessment for Goal 5 is an A-.

## **Goal 6.0 Deliver Efficient, Effective, and Responsive Business Systems and Resources that Enable the Successful Achievement of the Laboratory Mission(s)**

### **Highlights by Objective:**

- 6.1 Provide an Efficient, Effective, and Responsive Financial Management System(s)
- Instituted paperless approval for subcontract and significant dollar vouchers in select scientific programs to conserve paper and staff time.
  - Created plan and purchased equipment to institute paperless transfer of voucher information to Iowa State University. The system includes image retention of vouchers instead of hard-copy storage. Proposed full implementation of document scanning is in FY2013.
  - Established teams to help users to get information in a more useful format for the user's particular area. During the implementation of Deltek most of the emphasis was on the business users so some reports needed revising for non-financial use.
  - Quarterly "Institutional Cost Reports" were continued in FY2012 and submitted to DOE. The Lab will participate in peer reviews related to ICR.
  - The Laboratory was awarded two ARPA-e projects that started in FY2012. ARPA-e projects have additional reporting requirements over and above normal DOE projects and systems were created to meet these requirements.
  - A newly hired accountant developed and implemented training material for Laboratory travelers to effectively comply with DOE regulations.

Based on the above information, the Laboratory assesses its Financial Management system activities as a B+.

- 6.2 Provide an Efficient, Effective, and Responsive Acquisition Management System
- Reviewed and updated terms and conditions for contractors performing work at the Laboratory site.
  - In the process of testing an improved purchasing request process to be implemented in FY2013.
  - The Purchasing Manager participated in a PERT review at FERMI Lab in preparation for a PERT review at Ames. The experience obtained at the FERMI review was very beneficial to help the Ames manager prepare for Ames' first PERT review.
  - A PERT Review at Ames Laboratory was conducted in June 2012. The PERT review results were found to be favorable and no observations of a significant nature were identified. The Purchasing System was approved for an additional 3 years, through September 30, 2015.
  - Implementing improvement processes as identified as a result of the PERT (Purchasing Review). Areas of emphasis include improving file organization, ensuring adequate price/cost analysis is conducted, developing a standard requirements checklist, improving communication with requestors, and evaluating workload and deploying the appropriate amount of resources to support the improvements within the Purchasing Department.
  - To date the Purchasing Department has documented more than \$300K of cost savings/cost avoidance in FY2012.
  - A Davis Bacon Compliance Assessment was conducted during FY2012. The Laboratory is working on corrective actions developed from this assessment and working with the Ames Site Office to make sure the Laboratory corrections are acceptable.

Based upon the above information, the Laboratory assesses Acquisition Management system activities as a B+.

- 6.3 Provide an Efficient, Effective, and Responsive Property Management System

- 100% of Sensitive Property was found and 99.9% of capital and accountable property was found in 2012.
- The Property Management Systems Manager attended training on the new property management requirements. The new order provides some flexibility in dealing with property but will require some internal adjustments before the property policy can be fully implemented. Policies and procedures will be written in 2013 to implement the new Property Management Order.

Based upon the above metrics, the Laboratory assesses its Property Management system activities as a B+.

#### 6.4 Provide an Efficient, Effective, and Responsive Human Resources Management System and Diversity Program

- Implemented and launched Halogen e-Appraisal, an electronic performance appraisal system.
  - A joint project between Human Resources, Information Systems and Document, Training and Records began in October 2011. Halogen went live on February 28, 2012 for the 2012 performance evaluation process. In September 2012, Human Resources completed the test phase for the 3 month new employee performance evaluation process. The official process is scheduled to begin on October 1, 2012.
- Formalized and published the Scientific and Technical Review process.
  - In conjunction with the Chief Research Officer, Human Resources completed and formally documented the process for the Scientific and Technical Review Committee (STRC) process. One of the significant changes to this process includes the addition of an HR representative to each of the Scientific and Technical Review committees when they are established. The new documents and committee structure were utilized in the first round of recommended promotions in the Summer and Fall of 2011 and proved to be a positive and successful enhancement.
- Continued partnerships with Iowa State University.
  - Due to a lack of resources within the ISU Recruitment and Employment area, Ames Laboratory HR was approached to buy out a portion of the Asst. Human Resources Manager's position for a period of time until additional staff could be hired. Beginning in late December, the assistant manager began working ten hours a week over in the ISU employment office. This arrangement ended March 30, 2012 and proved to be very beneficial to Ames Laboratory and ISU.
- Hiring a new Program Coordinator
  - In June 2012, Human Resources hired a new Program Coordinator to design, develop and administer HR focused employee educational and development programs. The position will provide counsel and support to programs in the areas of performance management, succession planning and employee development.
- Documents, Training and Records
  - The Laboratory's Content Management system was expanded to include lab research notebooks and ESH&A records. Electronic capture of research documentation provides a much more stable and long-lasting archival format and enables researchers to conduct their work with much less disruption due to records management processes.
- As the result of targeted advertisements, the Ames Laboratory improved the overall diversity of applicants in our pools for open positions.
  - The increase in the diversity of pools can be directly attributed to the increased number of sites in which the Laboratory is advertising its open positions. Of the 39 filled positions between October 1, 2011 and September 30, 2012, we had over 748 applicants who declared their race and ethnicity; however white applicants made up 63% of our pools during the reporting period.
- 100% of hiring managers completed the on-line training on "Invite Diversity".

- We have been able to maintain 100% participation. Hiring managers are required to complete this course once every two years. The course is designed to help search committee members understand the importance of diversity and steps on how to diversify their applicant pools.
- An ongoing objective of the Ames Laboratory is to recruit and hire a diverse, excellent workforce, increase ethnic diversity of the workforce by 25%, increase women in the scientific and engineering workforce to 25%, and increase women in the overall workforce to 40%. As of September 1, 2012, our percentages included: ethnic minorities: 30.4% (up from 28.4%); women in the scientific and engineering workforce: 17.6% (down from 18%); and the percentage of women in the overall workforce dropped from 29.5% to 29.2%.

Based upon the above information and metrics, the Laboratory assesses its Human Resources and Diversity activities as an A-. Human Resources did not have notable outcomes for 2012 but did exceed expectations by implementing Halogen for both the annual performance appraisal process and a three month evaluation process for new hires. The hiring of the new program coordinator has also accelerated efforts on succession planning and strategic hires.

6.5 Provide Efficient, Effective, and Responsive Management Systems for Internal Audit and Oversight; Quality; Information Management; Assurance System and Other Administrative Support Services as Appropriate.

Information Services

- The FY2013 IM plan was prepared and strategies in place by September 30, 2012 with five goals identified in the FY2013 plan.
  - The HP3000 conversion project is complete.
  - For Maximo Enhancements, the software for capturing configuration data for IT assets was implemented on a test server and preventative maintenance requests continue to be tested.
  - Cognos 10 for Reports and Planner was implemented in a test environment.
  - The new web developer was hired and progress began on the web redesign.
  - For Network Infrastructure, the 10 gigabit components were purchased and the single mode fiber pull and termination is complete.
  - The Forms Routing/Workflow team met and prepared a draft summary document to be submitted to the Chief operations Officer.

Internal Audit

Internal Audit provided the following audit reports during FY2012:

- Statement of Costs Incurred and Claimed (SCIC): There was a total of \$2,427.79 of questioned costs from a \$4,976,349.75 sample. The sample was 14.64% of the total population of costs claimed of \$33,992,821.
- Financial Statement Review: Relative to Ames Laboratory statement, for the Fiscal 2011 time period Audit found compliance o the practices entailing general ledger account balances reconciliations being accomplished and compliance to reconciliation practice pertaining to review of DOE-generated statements in comparison to the internal statements for Ames Laboratory.
- Royalty Receipts Review : This audit was completed with the objective of verifying the net to share for one particular case for the ISURF fiscal period ending 6/30/2011.The case was #1732, Lead-Free Solder Alloy based on Tin-Silver-Copper. The total income indicated on the report was \$7,806,335.58. The total net to share for this case was \$3,344,991.76. The opinion of Audit was that the net to share

for Ames Laboratory was appropriate, in conjunction with the method and fees established by ISURF and approved by DOE.

- Work for Others: The opinion of the review was that internal controls are adequate and working as intended to ensure that Work for Others processes are ensuring compliance to requirements and that the best interests of the Laboratory are being realized and advanced through Work for Others' endeavors.
- Also, Internal Audit was active in reviewing physical inventories including storeroom inventories and physical inventories of equipment assets and reviewing the reasonableness of adjusting items. Audit also maintained follow up on past issues and we reviewed the relevant evidence of those agreements that were closed.
- We completed all of the audits indicated on the Approved Audit Plan for Fiscal 2012. We also tracked all corrective actions as coming forth from audit reviews until appropriate evidence of the action taken was verified.

#### Assurance System

- Ames hosted its Contractor Assurance Peer Review in November, 2011. The team noted in the final summary paragraph of the peer review team's report:  
*"The observations noted in this report indicate that the key elements of the CAS are in place and functioning as intended.... In its present state, the Ames Lab CAS is delivering benefits and positive impacts, and has strengthened the foundations of the partnership among ISU, AMSO and Ames Lab."*
- The partnership including Iowa State University, Ames Laboratory and the Ames Site Office have determined which opportunities for improvement of the Contractor Assurance System will provide the most cost-benefit and will focus on those two (EC identify most pressing risks, EC identify most useful metrics to use as key indicators). The Laboratory, ISU leadership, and Ames Site Office management will work on these issues together.
- The Laboratory and the AMSO have designated reviews where the two organizations partner to reduce the amount of intrusion on the focus area. This is a result of continuing CAS focus from both organizations.

#### Public Affairs

- Public Affairs hosted a media event for Ames Laboratory associate Danny Shechtman 2012 Nobel Laureate in Chemistry, in February 2012. Media from all major Iowa networks were in attendance, including Iowa Public Radio, WOI-TV, and the Des Moines Register.
- Public Affairs' efforts to promote scientific research at the Ames Laboratory have culminated in 204 media hits in newspaper, radio, television, e-zine outlets, etc. Examples of placements include the LA Times, New York Times and National Public Radio, Time magazine's Techland blog, local outlets like the Des Moines Register, Iowa Public Radio, and the Ames Tribune, and scientific outlets such as Greenwire, Scientific Computing and PhysOrg.
- Public Affairs promoted the Ames Laboratory's technology transfer efforts by publicizing the formation of spinoff company, Iowa Powder Atomization Technologies (IPAT), with a video, local media online and newspaper media placements, and a national profile on the technology and company. IPAT subsequently won the DOE's America's Next Top Energy Innovator Challenge award.
- Ames Laboratory and several of its scientists were in the spotlight at the PBS television series two-hour special on NOVA, "Hunting the Elements," in April 2012. Interviewed were senior physicist Paul Canfield, senior metallurgist Karl Gschneidner, senior metallurgist Bill McCallum and Materials Preparation Center Director Larry Jones.

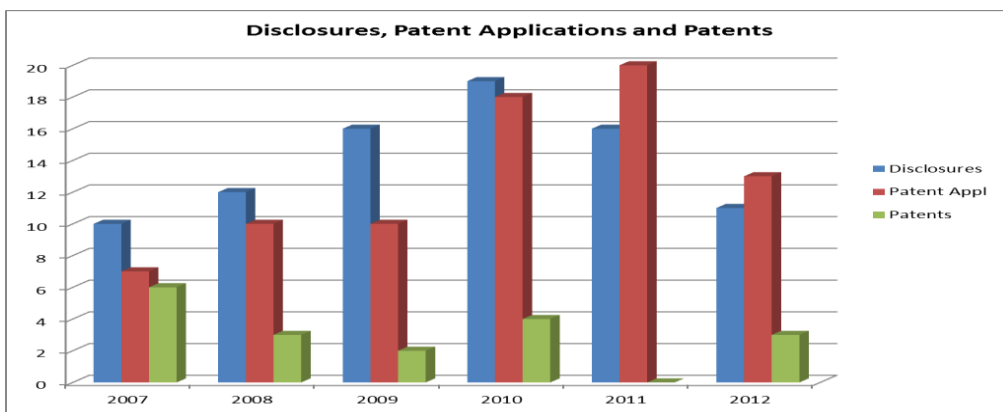
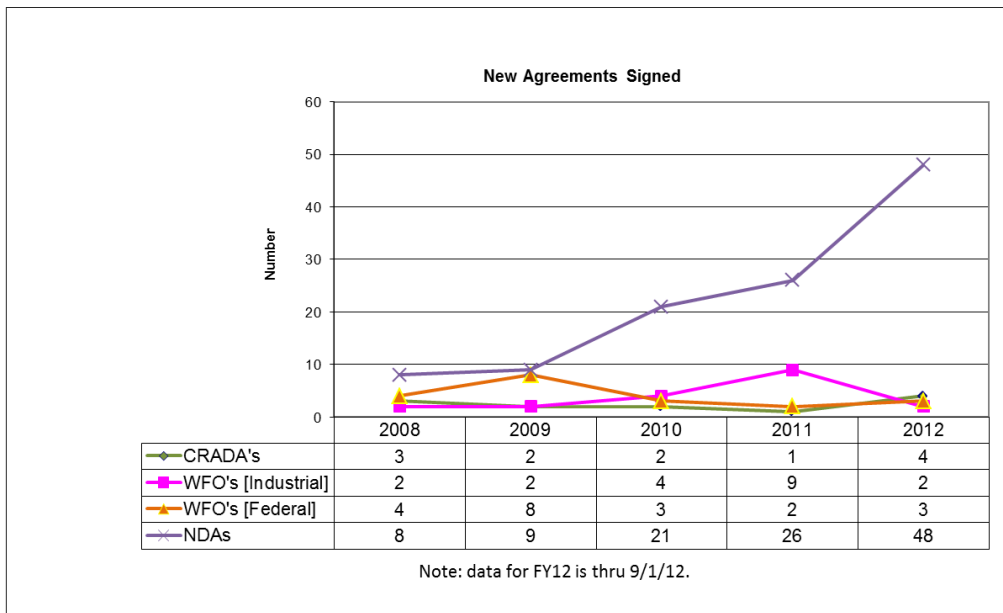


- Senior Metallurgist Iver Anderson was a guest on Iowa Public Radio's program "The Exchange" in January 2012 to talk about lead-free solder.
- Two needy charities were the recipient of approximately \$4,400 raised during the Ames Laboratory's annual Holiday Auction in December 2011.
- The Ames Laboratory exceeded its 2011 United Way goal, raising \$10,568, more than 105% of its goal.
- Public Affairs posted 13 "Ames Laboratory 101" and other videos to You Tube in FY2012. Of those videos, some of the most popular videos have been on the lead-free solder, rare-earth materials, and Iowa Powder Atomization Technologies.
- The Ames Laboratory's effort to produce alternatives to traditional rare-earth magnets were featured in a story in the New York Times in April 2012. Ames Laboratory's rare-earth work has also appeared in stories in National Geographic, the Philadelphia Inquirer, Greenwire and online outlets.

Based upon the above information and metrics, the Laboratory assesses its Efficient, Effective, and Responsive Management Systems for Internal Audit and Oversight; Quality; Information Management; Assurance System and Other Administrative Support Services activities as a B+.

#### 6.6 Demonstrate Effective Transfer of Technology and Commercialization of Intellectual Assets

- Worked on the Committee to get the Accelerated Commercialization of Technologies (ACT) Agreement accepted. Ames Laboratory is one of the pilot labs for this agreement.
- Earned Royalty Income (royalty income based on sales of products) from the 2011 DOE Datacall report once again placed AMES as the top DOE ERI generating Laboratory.
- For FY2011, Ames Laboratory inventions generated \$9,174,898 in royalty income which equates to \$766,879,618 in sales. The total represents over \$22 of economic activity for every dollar spent by the Laboratory in FY2011. Based upon an estimated Laboratory budget, we expect royalty income to be close to the FY2011 number.
- Developed TT Milestones and the IP Management Plan for the newly funded ARPA-E project where Ames Laboratory is the Lead.
- A Start-up Company, Iowa Powder Atomization Technologies ("IPAT"), that has an option to license Ames Laboratory technology under the America's Next Top Energy Innovator was 1 of 3 winners in the ANTEI Challenge. The company founders, a key inventor and the Associate Laboratory Director attended the ARPA-E Summit in February and met with Secretary of Energy Chu. Secretary Chu also presented the company, Iowa Powder Atomization Technologies, with a plaque during the Summit and spoke of the technology during his presentation. IPAT is currently in final negotiations for a license to the optioned technologies. In addition, IPAT was awarded first prize in the 2012 John Pappajohn Iowa Business Plan Competition, announced September 27, 2012.
- The Laboratory developed a formal Memorandum of Understanding (MOU) Plan in compliance with DOE requirements.
- The Laboratory:
  - Submitted 63 out of cycle proposals
  - Entered into 5 new WFO agreements (3 with a Federal Agency and 2 with non-federal partners)
  - Initiated and signed 6 WFO amendments
  - Executed 4 new CRADA and 9 Amendments;
  - Initiated and/or executed 48 NDAs;
  - Entered into 2 MOUs; and 4 MTAs.
  - Entered into 1 IPA; and 2 TSAs.
  - ISURF entered into 1 License.



The Laboratory assesses its technology transfer activities as an A-. This is based on the Laboratory's leadership position on transferring technology as evidenced in its leadership position in earned royalty income and the recognition received from IPAT winning one of America's Next Top Energy Innovator awards; and the leadership shown by the Associate Laboratory Director for Sponsored Research Administration and her staff as they worked to set up the new ACT program and handled the influx of new NDAs driven by the increased interest in materials generally and the rare earth materials situation specifically.

### Notable Outcomes

**6A: Ames Laboratory subject matter experts for Work For Others (WFO), Intellectual Property (IP), Cyber Security, Safeguards & Security (S&S) and Science will work together to develop an integrated plan to address potentially sensitive information developed during scientific research, including WFO. (Objective 6.6)**

- A team was formed consisting of individuals from IS/Cyber, export control, intellectual property, foreign visits and assignments, safeguards and security and the scientific divisions to integrate various

Sensitive Information activities into one concise plan. Much of the processes performed within each functional area was already documented and was culled out of the various approved Plans and Policies and consolidated into one cohesive document. Each functional area worked on identifying what documents in their area applied and provided them to the Associate Laboratory Director for incorporation into the Integrated Technology and Security Assurance Plan. The Plan has had AMSO review and is now undergoing internal approvals.

**6B: Implement planned improvements resulting from the proposal submission improvement process review committee conducted during FY2011. Areas of emphasis should include timeliness and quality of packages sent to DOE. (Objective 6.6)**

- The proposal committee met three times to work on the electronic routing of our proposals, deployment of spreadsheet models to the research staff for building initial budget formulation, and concurrent review/approval processes. Members are currently looking at software packages that may meet our needs regarding electronic routing, but several that have been looked at are very expensive. The team has discussed with ISU the possibility of utilizing their system, but currently this does not seem a viable option. However, the possibility exists that when ISU fully implements Quali Coeus, their new business system, that we may be able to utilize that system; current estimates for ISU's proposal routing using Quali Coeus is 2-3 years. In the meantime, we are looking at alternatives.
- Recent indications from the AMSO, during the quarterly meetings/teleconferences between AMSO and OSRA, are that the timeliness and quality of proposals for DOE approvals have improved. Some anticipated reorganization within the OSRA, as well as the newly created Proposal Team should provide additional process improvements in this area.
- As one of FY2011 Proposal Review Committee recommendations, the Proposal Team, created in FY2012 as a pilot test to see if such a team would help improve our proposal submissions and to coordinate preparation and approvals of large multi-PI/Team proposals worked on the Ames Laboratory lead CMI proposal. The Laboratory Director and the Proposal Committee is in the process of determining the effectiveness of the Team and the next steps in internal improvements of the proposal process.

Both Notable Outcomes 6A and 6B were met.

The Laboratory's overall assessment for Goal 6 is a B+.

## Goal 7.0 Sustain Excellence in Operating, Maintaining, and Renewing the Facility and Infrastructure Portfolio to Meet Laboratory Needs

### Highlights by Objective:

- 7.1 Manage Facilities and Infrastructure in an Efficient and Effective Manner that Optimizes Usage, Minimizes Life Cycle Costs, and Ensures Site Capability to Meet Mission Needs
- The Spedding Auditorium renovation is complete. This provides state of the art conference and presentation space. The facility has extensive A/V, networking, and distance learning capabilities. It provides great flexibility to support the different types of meetings and presents an excellent image of the Laboratory to visitors and staff.
  - The Laboratory initiated a project to upgrade its network infrastructure to 10-Gig transmission speeds. To date the equipment has been purchased and the fiber has been pulled and terminated. The remainder of the equipment will be installed and configured in FY2013.
  - As part of the HVAC upgrade in Spedding Hall, the entire drain line in the basement had to be replaced. The drain was contaminated and had to be replaced and sealed as new drains were installed. This portion of the project was completed with minimal disturbance of the research effort being conducted in the building. If the replacement was not done as part of the planned project, a future failure of the drain line would cause a prolonged outage which would have a much greater impact on the research being performed in the building.
  - A tuck pointing project was performed on a section of the Spedding Hall over the front entry to repair an area with significant cracks and freeze-thaw damage. Deferring the project would have run the risk of a failure that would cause bricks to fall over the entry. A section of parapet was removed and rebuilt and a significant area of exterior masonry in that section was replaced. The height of the parapet was reduced in order to reduce the re-build cost and to simplify the structure to decrease future maintenance.
  - Sustainability
    - The project to seal the leaks in fume hood stacks in Spedding Hall has completed over 50% of the work. To date the project has decreased the exhaust quantities by 12,000 cfm generating energy savings of \$40K per year.
    - The Laboratory has developed plans and secured funding for the installation of a hot aisle/cold aisle air containment system to enhance the effectiveness of the data center in Harley Wilhelm Hall.
    - Two 80 KVA UPS units serving a data center have been upgraded to boost operating efficiency from an estimated 92% to approximately 99%. Estimated savings are approximately \$4K per year.
    - Lighting fixture upgrade designed to improve fixture ballast factors have been performed on approximately 1,000 fixtures to date with estimated annual savings of approximately \$4K in electrical costs.
    - Project scope and specifications were prepared and backroom equipment purchased and installed for a project to migrate administrative desktop computing away from individual PCs to a thin client system. Preliminary estimates place energy saving at 80%+ compared to traditional desktop PCs.
    - Ames Laboratory employees can utilize the municipal mass transit system eliminating personal use of automobile and reducing the demand for parking on campus. ISU supports the system financially so that all Ames Laboratory employees can use the system on campus for free.
    - Ames Laboratory designated preferred parking spots for hybrid vehicles to encourage their usage.

- The ISU Heating Plant, that provides steam and chilled water to the Ames Laboratory, continues to investigate the feasibility of alternate fuels for their boilers. Wood-based bio-fuel has been tested in the plant and permits for its use have been obtained, however the fuel is not economically competitive.

Based upon the above information, the Laboratory assesses its management of existing facilities and infrastructure as a B+.

#### 7.2 Provide Planning for and Acquire the Facilities and Infrastructure Required to Support the Continuation and Growth of Laboratory Missions and Programs

- The Laboratory continues to make progress on the Sensitive Instrument Facility. The 2011 Lab Plan identified this as one of the critical facilities and infrastructure projects needed to support Laboratory missions and programs. Since then, funding totaling \$5.5M has been received from the Office of Science for the project. The Site Evaluation Study has been completed by outside consultants and the procurement of A/E design services is complete. The Laboratory has received its first deliverable from A/E, the Program Report and is working on the next set of deliverables.

Based upon the above information, the Laboratory assesses its facility acquisition planning as a B+.

#### Notable Outcomes

##### **7A: The Mission Readiness Leadership Team will prepare a written evaluation of the review team's opportunities for improvement, including a plan of action for those recommendations deemed beneficial to implement. (Objective 7.1)**

- The Mission Readiness Peer Review was performed July 26-28, 2011. The review concluded that the Laboratory met the four mission readiness objectives and identified strengths as well as seven opportunities for improvement (OFI). The Mission Readiness Leadership Team evaluated the OFI's and generated actions that provided value-added improvements. Some of the actions to address of the OFI's were incorporated directly within the Mission Readiness Process or in Laboratory Operations. They were incorporated in the mission readiness activities in FY2012. Three of the seven OFI's require no further actions. The review also identified actions items to address the remaining OFI's that are to be completed in FY2013 and FY2014. The review and action plan was formalized and submitted to the Ames Site Office by letter on September 11, 2012.

Some of the notable responses to the OFI's are listed below:

- During the FY2012 mission readiness process, issues and needs were identified and placed into a database that documents the issue or need, the affected program, the stakeholders, the person identifying the issue, the infrastructure elements involved and the status. This information is used for feedback to directors and managers to help them track status and to help in planning for future recommendations.
- The Ames Laboratory has leveraged its relationship with ISU to utilize their capabilities and resources to benefit the Laboratory. The Ames Laboratory facilities manager and staff have worked with ISU Facilities Planning and Management (FP&M) on the A/E selection and design input for the Sensitive Instrument Facility. We are utilizing ISU's web-based tool Centric Project to facilitate collaboration

and communication between team members for the project. This tool allows team members, such as architects, engineers, contractors, and university constituents to access and collaborate on all of the various types of information generated for a project.

- The Ames Laboratory teamed with ISU FP&M personnel who provided assistance to recover from an electrical fire that damaged switchgear in Metals Development. ISU engineering staff and high voltage electricians assisted in the emergency response and in the recovery. With ISU and Ames Laboratory personnel working together, the damaged equipment was removed from the enclosure and the electrical feed was rerouted so that full electrical service was restored before the end of the day.

Notable Outcome 7A was met.

The Laboratory's overall assessment for Goal 7 is a B+.

## **Goal 8.0 Sustain and Enhance the Effectiveness of Integrated Safeguards and Security Management (ISSM) and Emergency Management Systems**

### **Highlights by Objectives:**

#### **8.1 Provide an Efficient and Effective Emergency Management System**

- Full participation emergency drill with Ames Fire Department Hazardous Material Team was performed on three consecutive days to enable participation for each fire department shift. Re-running the exercise on consecutive days allowed greater participation by the Ames Laboratory Emergency Response Team members, giving team alternates excellent training experience. Interactions with local spill response entities during drills brought about changes in the Laboratory's Emergency Management Plan to provide better alignment with Incident Command System guidance.
- The Laboratory has identified an individual to take over the Emergency Coordinator duties. This individual has been working with the current Emergency Coordinator and reviewing the directives, policies and procedures in order to become familiar with the role. He has been assigned the role of alternate Incident Commander and participated in the drill described above. It is our goal to turn over the role permanently in FY2013.

Based upon the above information, the Laboratory assesses its Emergency Management activities as an A-. This is based on the efforts to organize and execute a 3 day emergency drill with the Ames Fire Department HazMat team and other local emergency response organizations. This event allowed all organizations to leverage the activity, learn from the experience and make improvements for coming emergencies. It also allowed the Ames Laboratory emergency team members to practice the various roles they are expected to fill. The event provided a great opportunity to build on our relationships within the Lab and within the emergency response community.

#### **8.2 Provide an Efficient and Effective System for Cyber-Security and National Security Systems (NSS)**

- The stateful, routing firewall was procured. The selected vendor was McAfee. The Cyber/IS staff received training on the new firewall.
- The Ames Laboratory conceptual baseline reflects the Office of Science S&S Baseline Level of Protection and establishes a basis for formulation and execution of S&S program efforts.
- Chris Strasburg was included in a successful Argonne National Laboratory proposal to work on a DOE Laboratory-wide cyber federated model to enhance cyber security at all laboratories. The work is scheduled to begin in FY2013.

Based upon the above information, the Laboratory assesses its Cyber-Security and NSS as a B+.

#### **8.3 Provide an Efficient and Effective System for the Physical Security and Protection of Special Nuclear Materials, Classified Matter, and Property**

- A physical protection system risk assessment was conducted at the Ames Laboratory in May 2012 by a team assembled by SC and HSS. The report indicates that the physical protection program at the Ames Laboratory provides a level of physical protection that is balanced, cost effective, and reasonable based on DOE Directives and the SC BLP. Five recommendations were identified and corrective actions are in progress.

- A topical appraisal of Materials Control and Accountability was completed in August 2012, opportunities for improvement were identified and corrective actions have been initiated.
- The Property Office is working with the Export Control Manager to identify High Risk Property, including Export Controlled Equipment. The Procurement Office has begun asking vendors to supply export control classification numbers, if applicable, for equipment on order.

The Laboratory assesses its Physical Security and Protection of Special Nuclear Materials, Classified Matter, and Property as an A-. This is based on the success of the risk assessment and the verification that the Ames Physical Protection program is balanced, cost effective and reasonable. The reviews were very positive about our program.

8.4 Provide an Efficient and Effective System for the Protection of Classified and Sensitive Information

- A team of subject matter experts worked together to develop an Ames Laboratory integrated plan to address potentially sensitive information developed during scientific research, including WFO (as reported under Notable Outcome 6A).

Based upon the above information, the Laboratory assesses its Protection of Sensitive Information as a B+.

**Notable Outcomes:**

**8A: Once the PCSP is released, complete a plan for transition of the security authorization to the risk management framework, establish milestones for implementation, and complete milestones that fall within FY2012. (Objective 8.2)**

- The PCSP was not released.
- The Risk Management Framework guidance was reviewed.
- For the low and moderate enclave, security controls were evaluated, opportunities for improvement were identified, and volatility assessment was performed.
- Discussion occurred with the Site Office staff. Periodic meetings will be held throughout FY2013 to discuss continuous monitoring processes.
- Began to develop processes for evaluating low and moderate security controls.

Notable Outcome 8A was met.

The Laboratory's overall assessment for Goal 8 is an A-.