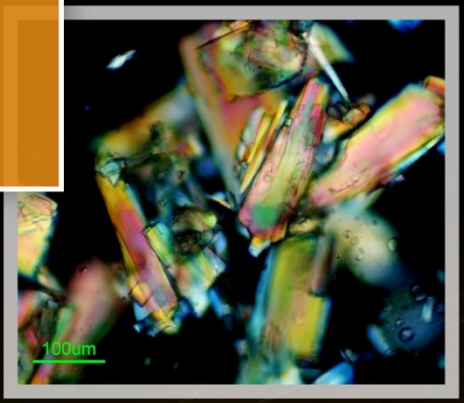
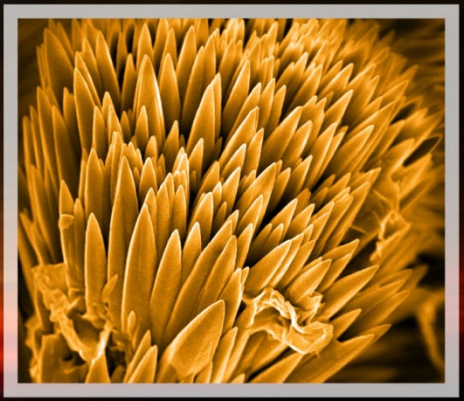
2013 Laboratory Plan





DISCOVERY *in Action*

Pacific Northwest
NATIONAL LABORATORY

Proudly Operated by **Battelle** *Since 1965*

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Acronyms and Abbreviations

ARM	Atmospheric Radiation Measurement Climate Research Facility
ACT	Agreements for Commercializing Technology
AML	Atmospheric Measurements Laboratory
ANL	Argonne National Laboratory
APEL	Applied Process Engineering Laboratory
ARRA	American Recovery and Reinvestment Act
ASCR	Advanced Scientific Computing Research
BER	Biological and Environmental Research
BES	Basic Energy Sciences
BNL	Brookhaven National Laboratory
BSEL	Bioproducts, Sciences, and Engineering Laboratory
CASS	Center for Advanced Supercomputing Software
CBRNE	chemical, biological, radiological, nuclear, or explosive
CD	Critical Decision
COR	charge-out rate
CSF	Computational Sciences Facility
CTA	Center for Transportation Analysis
CSIL	Chemical Sciences and Imaging Laboratory
DARPA	Defense Advanced Research Projects Agency
DHS	U.S. Department of Homeland Security
DNDO	Domestic Nuclear Detection Office
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
EERE	Office of Energy Efficiency and Renewable Energy
EIA	Electronic Industries Alliance
EIOC	Electricity Infrastructure Operations Center
EM	Office of Environmental Management
EMSL	Environmental Molecular Sciences Laboratory
EPA	U.S. Environmental Protection Agency
FE	Office of Fossil Energy
FTE	full-time equivalent
GA	global array
GHG	greenhouse gas
GPP	General Plant Project
gsf	gross square feet
HPSB	high performance sustainable building
HS	Office of Homeland Security
IGPP	Institutional General Plant Project
iRESM	integrated regional Earth system model
JGCRI	Joint Global Change Research Institute
LBNL	Lawrence Berkeley National Laboratory
LDRD	Laboratory Directed Research & Development
LSL-II	Life Sciences Laboratory II
MOF	metal-organic framework
MNS	Mission Need Statement
MS	mass spectrometry
MSL	Marine Sciences Laboratory
NASA	National Aeronautics and Space Administration
NE	Office of Nuclear Energy
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NNSA	National Nuclear Security Administration
NOAA	National Oceanic and Atmospheric Administration
NRC	U.S. Nuclear Regulatory Commission
NTNFC	National Technical Nuclear Forensics Center
OE	Office of Electricity Delivery and Energy Reliability
ORNL	Oak Ridge National Laboratory
PICC	PNNL Institutional Computing program
PLM	polarized light microscope
PNNL	Pacific Northwest National Laboratory
PNSO	Pacific Northwest Site Office
PSF	Physical Sciences Facility
PSL	Physical Sciences Laboratory
PV	photovoltaic
RCL	Radiation Calibration Laboratory
REC	renewable energy certificate
RPL	Radiochemical Processing Laboratory
RTL	Research Technology Laboratory
SC	Office of Science
SNL	Sandia National Laboratory
STEM	Science, Technology, Engineering, and Mathematics (education)
STXM	scanning transmission x-ray microscopy
TEM	transmission electron microscopy
USACE	U.S. Army Corps of Engineers
UW	University of Washington
WFO	work for others
WSU	Washington State University

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SELECTED AWARDS AND RECOGNITION

PNNL Teams Receive DOE Secretary's Honor Award

Three teams of PNNL researchers were presented Honor Awards from Energy Secretary Chu for their impactful efforts on high-priority projects. The teams were recognized for their work related to the Deepwater Horizon oil spill in the Gulf of Mexico, the tsunami-damaged Fukushima Daiichi Power Plant in Japan, and for their work to transport and secure spent fuel from a Kazakhstan nuclear power plant. The Honor Awards represent the highest level of non-monetary recognition given to DOE federal and contractor employees.

Julia Laskin – Rising Star Award

Julia Laskin is the recipient of the inaugural Rising Star Award from the Women Chemists Committee of the American Chemical Society. This award honors 10 women in the chemistry enterprise who have made outstanding contributions in their fields of study. Julia was selected for her work in mass-spectrometry, a field in which she is recognized as one of the preeminent authorities of novel techniques and their application to important scientific problems.

Wei-Jun Qian – Recipient of PECASE Award

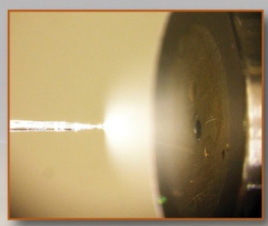
Wei-Jun Qian has been recognized with a 2011 Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor given by the U.S. government for early career scientists and engineers. Qian, who was recognized for his work in proteomics, is using mass spectrometry to research more accurate methods to measure protein concentrations. This information could help make the biological production of biofuels and other bioproducts more efficient.

Federal Laboratory Consortium Award

PNNL is the recipient of three 2011 Excellence in Technology Transfer award from the Federal Laboratory Consortium (FLC). As the recipient of 74 FLC awards, PNNL has been recognized with this honor more than any other federal laboratory since the program began in 1984.

- IncubATR™-the Live-Cell Monitor
- Low Noise Quantum Cascade Laser Current Controller
- Propylene Glycol from Renewable Sources

R&D 100

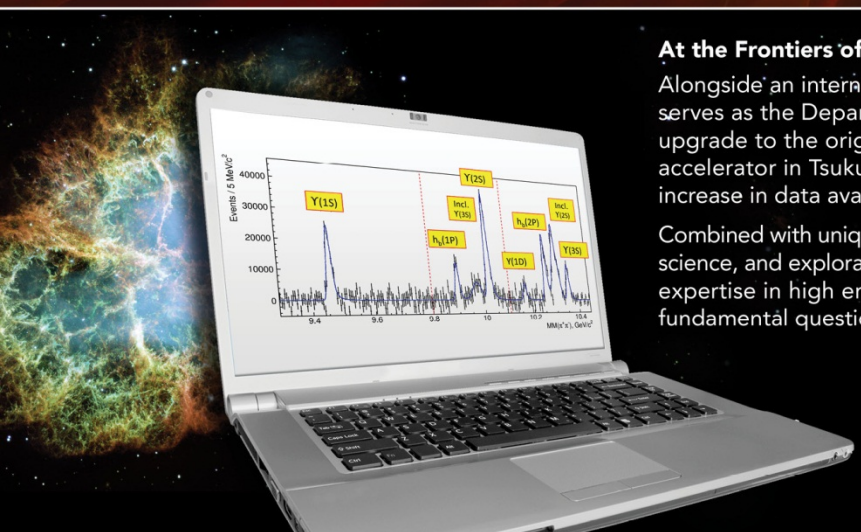


The R&D 100 Awards honor the inventors of the 100 most technologically significant products and advancements every year as determined by R&D Magazine. To date, PNNL has received 87 of these covered awards, including two in 2011.

- Array Detection Technology for Mass Spectrometry
- Dynaforge—A Solid-State Dynamic Powder Compaction Process for Production of High-Performance Tools and Dies

Sam Payne – DOE Early Career Research Award

Sam Payne is a recipient of the DOE Early Career Research Award for his research in the area of improved sensitivity and utility of metaproteomics analysis. Sam will apply the award towards advancing research in identifying proteins that could be used in biofuel production.



At the Frontiers of Particle Physics Research

Alongside an international group of high-energy physicists from 17 countries, PNNL serves as the Department of Energy's lead laboratory for the Belle II project, an upgrade to the original multilayered particle detector at Japan's KEK particle accelerator in Tsukuba, Japan. The outcome is estimated to produce a 50-fold increase in data available for precision studies and discovery science.

Combined with unique capabilities in ultra-low-background radiation detection, neutrino science, and exploration of dark matter research, Belle II contributes to PNNL's growing expertise in high energy physics which aims to help researchers answer the most fundamental questions about the nature of the universe.

Sub-atomic Breakthrough. *Physicists trying to identify all the subatomic particles thought to exist have found another two (the peaks labeled h_b). These newly identified particles are two new pieces of the puzzle that will help researchers understand what makes the universe tick.*

1.0 Mission/Overview

The Pacific Northwest National Laboratory (PNNL) is a U.S. Department of Energy (DOE) Office of Science (SC) laboratory located in Richland, WA with an enduring mission to transform the world through courageous discovery and innovation. Our vision inspires and enables the delivery of world-leading science and technology in the following areas:

- controlling interactions across scales to enable scalable synthesis
- efficient and secure electricity management from generation to end use
- coupling earth and energy systems for sustainability
- signature discovery and exploitation for threat detection and reduction
- *in situ* chemical imaging and analysis
- accelerating innovation and discovery and transforming the conduct of science in the Environmental Molecular Sciences Laboratory (EMSL)
- simulation and analytics.

PNNL also has two national scientific user facilities: EMSL, providing integrated experimental and computational resources for discovery and technological innovation; and the Atmospheric Radiation Measurement Climate Research Facility (ARM).

Established in 1965 with 2200 employees and facilities supporting Hanford Site operations, PNNL focused on expanding nuclear fuel cycle research, developing advanced reactor designs and materials, fabricating and testing novel reactor fuels, and monitoring and protecting human health and the environment. Today, PNNL is a leading multidisciplinary national laboratory with a long-standing reputation for advancing scientific frontiers through world-class research and development.

PNNL is operated by Battelle Memorial Institute, a private, non-profit, science and technology enterprise that explores emerging areas of science, develops and commercializes technology, and manages laboratories. Total PNNL cost for FY 2011 was $876.3M. PNNL customers include DOE, the National Nuclear Security Administration (NNSA), the U.S. Department of Homeland Security (DHS), and other federal agencies. Details on specific Work for Other agencies are provided in Appendix 1.

2.0 Laboratory at a Glance

Location: Richland, WA
Type: Multiprogram Laboratory
Contract Operator: Battelle Memorial Institute
Responsible Site Office: Pacific Northwest Site Office (PNSO)
Website: http://www.pnnl.gov/

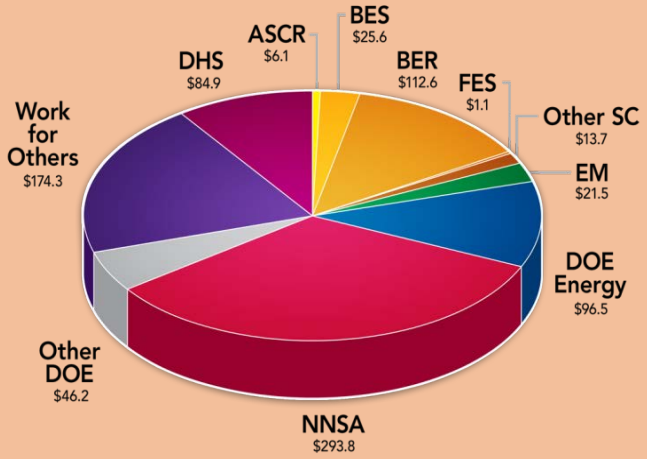
Physical Assets

- 346 acres DOE, 268 acres Battelle, 19 DOE Buildings, 96 Total buildings
- 830,803 gross square feet (GSF) of DOE-owned, active operating buildings
- Replacement Plant Value: $409,483,904 *(see Section 6, Table 2)*
- 1,111,048 GSF in 36 leased facilities
- 390,992 GSF in 41 Battelle facilities

Human Capital

- 4180 FTE Employees (2411 Direct; 1769 Indirect)
- 3 Joint Appointments
- 191 Postdoctoral Researchers
- 205 Undergraduate
- 171 Graduate Students
- 2414 Facility Users (750 EMSL; 1664 ARM)
- 40 Visiting Scientists (EMSL)

FY 2011 Funding by Source *(Cost Data in $M)*:



FY11 Total Laboratory Operating Costs (excluding Recovery Act):	$876.3M
FY11 Total DOE/NNSA Costs:	$617.2M
FY11 WFO (Non-DOE/Non-DHS) Costs:	$174.3M
FY11 WFO % of Total Laboratory Operating Costs:	28%
FY11 Total DHS Costs:	$84.9M
Recovery Act Costed from DOE Sources in FY 2011:	$68.6M

3.0 Current Laboratory Core Capabilities

PNNL has ten acknowledged core capabilities (Figure 1). Each is a powerful combination of people, equipment, and facilities nurtured through programmatic, institutional, and corporate investments. PNNL makes discretionary investments in these core capabilities and other strategically important areas to respond to emerging and future national needs. Current investments are designed to expand the Laboratory's capabilities in multi-modal imaging, power grid science and technology, computational science, earth systems science, microbiology, and materials science.

Several PNNL core capabilities have matured into world-class research programs. For example, PNNL is widely recognized as a world leader in proteomics, drawing on core capabilities in chemical and molecular sciences and biological systems science. Other capabilities have led to world-class research in catalysis, climate research, subsurface science, and radiation detection.

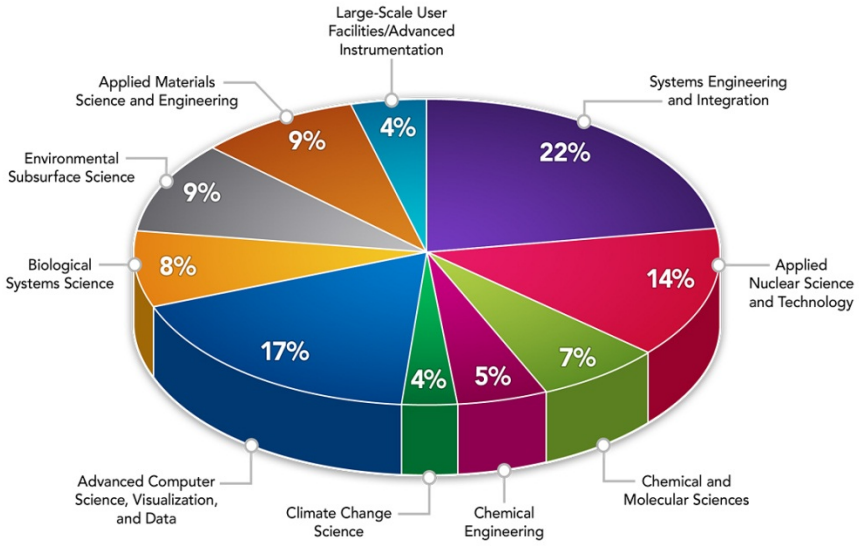


Figure 1. PNNL Technical Staff by Core Capability

One of PNNL's strengths is the ability to bring multiple capabilities to bear on complex scientific and technological challenges. This approach, combined with our focus on accelerating scientific discovery and innovation and deploying solutions, is evident in the core capability descriptions, primary funding sources, and supported missions that follow. See Appendix 2 for the Mission Area key used in the core capability descriptions.

3.1 Chemical and Molecular Sciences

PNNL is a national leader in chemical and molecular sciences. This core capability advances the understanding, prediction, and control of chemical and physical processes in complex, multiphase environments. PNNL has domain expertise in condensed phase and interfacial molecular sciences, catalysis science, computational and theoretical chemistry, geochemistry, separations and analysis, actinide science, self-assembled nanomaterials, and defects in materials.

This capability is the basis for PNNL's computational chemistry software application (NWChem), which is used worldwide to solve large molecular science problems efficiently using computing resources ranging from high-performance parallel supercomputers to workstation clusters. The Laboratory has made significant contributions in condensed phase and interfacial molecular science, fundamental catalysis science, and geochemistry. PNNL has the largest fundamental research effort within the national laboratory system in these areas, and this success has resulted in the establishment of the Institute of Interfacial Catalysis and the award of an Energy Frontier Research Center in Molecular Electrocatalysis from DOE's Basic Energy Sciences (BES) program. PNNL has also developed Northwest–Infrared, a comprehensive vapor phase spectral library for chemical-sensing applications, and made it available to researchers worldwide. This capability supports 148 staff scientists and engineers housed in the Physical

Sciences Laboratory (PSL), EMSL, and other facilities. This capability contributes to and benefits from EMSL's state-of-the-art resources.

The chemical and molecular science capability forms the basis for PNNL's fundamental science programs in condensed phase and interfacial molecular sciences, chemical analysis, computational chemistry, geochemistry, and catalysis science. Applied programs include improved energy technologies, catalysis and reaction engineering, hydrogen storage, biomass conversions, environmental remediation, and carbon capture and sequestration. This capability is funded through programs in SC (BES and Biological and Environmental Research [BER]), DOE's Office of Environmental Management (EM; environmental remediation), Energy Efficiency and Renewable Energy (EERE; geothermal; biomass; hydrogen, fuel cells, and infrastructure technology), Fossil Energy (FE; carbon- and co-sequestration), and NNSA (nonproliferation). This capability enables PNNL to advance DOE's missions in scientific discovery and innovation (SC 7, 8, 9, 11, 16), energy security (ES 5, 8, 9), environmental management (EM 2, 3), national security (NNSA 2), and homeland security (Office of Homeland Security [HS] 1, 2, 3, 5, 6).

3.2 Chemical Engineering

PNNL is recognized internationally for its chemical engineering core capability. This capability applies chemical research and engineering across molecular to engineering-scale problems and demonstrations, translating scientific discovery into innovative processes for advanced energy and environmental systems. PNNL's strength in chemical engineering is derived from its scientific foundations in molecular, biological, nuclear, and material sciences and engineering. An important feature of this capability is its ability to deliver continuous, high-throughput, efficient and cost-effective processing solutions with supporting equipment and controls, often incorporating several advanced individual processes and systems. The Laboratory has domain expertise in applications of catalysis for biomass and fossil fuel conversion; separations and waste immobilization for nuclear waste processing; online sensing of nuclear, chemical, and biological materials; clean hydrocarbon processing and emissions; micro-technology-based chemical engineering and micro-chemical reactor technology; fluid dynamics for complex fluids; electrochemistry; and carbon capture.

In collaboration with Washington State University (WSU), PNNL established the Bioproducts, Sciences, and Engineering Laboratory (BSEL), including state-of-the-art catalytic reactors and bio-processing laboratories to convert biomass into viable products such as biofuels and chemicals. PNNL has more than 108 scientists and engineers supporting this capability, along with facilities (some of which are unique) for radiochemical processing and process engineering, including the BSEL, PSL, Radiochemical Processing Laboratory (RPL), and Applied Process Engineering Laboratory (APEL).

The chemical engineering capability forms the basis for PNNL's programs in emission catalysis, hydrogen fuel safety and storage, hydrogen storage and carbon capture, biomass conversion, clean coal technologies, fuel cell development (including solid oxide fuel cells), tactical energy systems, used nuclear fuel and waste processing, and waste forms. It is funded through programs in EERE (geothermal; biomass; hydrogen, fuel cells, and infrastructure technology; and vehicles), FE (clean coal, hydrogen and other clean fuels, and carbon capture), DOE's Office of Nuclear Energy (NE – used fuel treatment), and EM (waste processing). This capability enables PNNL to advance DOE's missions in scientific discovery and innovation (SC 11), energy security (ES 6, 7, 8, 9), environmental management (EM 2, 3), national security (NNSA 2), and homeland security (HS 3, 6, 7, 8, 9).

3.3 Biological Systems Science

PNNL is recognized internationally for its biological systems sciences capability, including leadership in proteomics, environmental microbiology, fungal biology and biotechnology. PNNL's multiple 'omic technologies are widely used in the broader BER Programs. PNNL's domain expertise

also includes cell biology and biochemistry, radiation biology, computational biology and bioinformatics, systems toxicology, bioforensics, and biodetection.

The Laboratory has demonstrated international leadership in proteomics and environmental microbiology, designing strategies for biorestoration of sites contaminated with heavy metals and radionuclides, predicting contaminant behavior in the subsurface, and a systems biology approach to microbial and algal systems relevant to DOE missions of bioenergy and climate change. PNNL's expertise in fungal biology has generated an in-depth understanding of the biological processes underlying efficient fungal bioprocesses that produce fuels and other chemicals. Supporting this capability are more than 173 scientists and engineers housed in the new Biological Sciences Facility, Computational Sciences Facility (CSF), BSEL, Marine Sciences Laboratory (MSL), 331 Building, and EMSL. PNNL is also a partner in the Joint Genome Institute, which provides large-scale genome sequencing and analysis for DOE missions.

The biological systems science capability enables PNNL to provide a systems-level understanding of biological systems involved in biomass conversion, radiation biology, biology of oxidative stress and signaling, environmental sustainability, carbon cycling and terrestrial biosequestration, biogeochemical transformation of environmental contaminants and nutrient including carbon, environmental microbiology, microbial ecology, and bioforensics and biodetection. The capability is funded through programs in SC (BER), EM (waste processing), EERE (biomass), DHS, National Institutes of Health (NIH), and the U.S. Environmental Protection Agency (EPA). This capability advances DOE's missions in scientific discovery and innovation (SC 12, 14, 15, 16), energy security (ES 8, 9), environmental management (EM 2), and homeland security (HS 3, 11).

3.4 Climate Change Science

PNNL is a national leader in climate change science, with expertise spanning the full range of disciplines and tools needed to understand and quantify complex interactions among the natural earth system, energy production and use, and other natural processes and human activities. This core capability includes activities ranging from measurements to multiscale models to integrated analyses of climate impacts and response options. PNNL has domain expertise in instrument development; cloud physics; atmospheric aerosol chemistry; cloud-aerosol-precipitation interactions; laboratory studies, field campaigns, and other measurement programs; atmospheric process modeling; regional and global climate and Earth system modeling; integrated assessment; and quantitative analyses of emissions, land use changes, and mitigation and adaptation scenarios. Increasingly, these tools and techniques are being integrated to yield new insights into coupled natural-human system dynamics—for example, PNNL's state-of-the-art integrated regional Earth system model (iRESM) includes high-resolution representations of the atmosphere, oceans, land surface hydrology, agriculture and land use, energy systems, and socioeconomics; includes a sophisticated uncertainty characterization and quantification framework; takes advantage of advanced computing and data management and visualization tools; and is being used to identify the regional impacts of climate change and evaluate different adaptation and mitigation options.

PNNL is internationally recognized for improving our basic understanding of the causes and consequences of climate change and for developing the data-driven regional and global modeling frameworks needed to predict changes in climate as well as in related human and environmental systems. More than 82 scientists and engineers support this core capability, including those housed in the Atmospheric Measurements Laboratory (AML) and MSL, those supporting the ARM User Facility, and those at the Joint Global Change Research Institute (JGCRI), a partnership between PNNL and the University of Maryland that focuses on understanding the interactions among climate, natural resources, energy production and use, economic activity, and the environment. PNNL scientists have made major contributions to a number of national and international assessments of climate change, including the Nobel Prize-winning Intergovernmental Panel on Climate Change.

The Climate Change Science capability provides the basis for PNNL's programs in atmospheric process research; earth system observations; integrated assessment of climate and related global changes; and climate and Earth system modeling and prediction. It is funded by programs in SC (BER and Advanced Scientific Computing Research [ASCR]), EERE (wind and water power technologies), FE (carbon- and co-sequestration), the National Aeronautics and Space Administration (NASA), EPA, and the National Oceanic and Atmospheric Administration (NOAA). This capability advances DOE's missions in scientific discovery and innovation (SC 1, 13, 15, 16), energy security (ES 16), and homeland security (HS 7, 9, 11).

3.5 Environmental Subsurface Science

PNNL is an international leader in environmental subsurface science. This core capability focuses on developing and applying the basic understanding of biogeochemical reactions, energy, and mass transfer to the prediction, assessment, mitigation, and design and operation of *in situ* environmental processes. PNNL has domain expertise in molecular-to-field scale biogeochemistry and reactive and multiphase transport modeling; laboratory-to-field scale geohydrology, surface water hydrology, and multiphase flow modeling; ecological assessment, management, and monitoring; human health and environmental risk assessment; and environmental systems technology development and deployment.

PNNL applies an iterative experimental and modeling approach to contaminant fate and transport at DOE sites, demonstrating its leadership at the Integrated Field Research Challenges located within the Hanford Site 300 Area and research focused on molecular scale biogeochemical processes, field relevant microsites, and transition zones. The Laboratory applies this expertise toward the protection of regional water sources and aquatic ecosystems affected by contaminated soils and groundwater, releases from waste disposal units, climate change mitigation, energy development, water use, and hydropower systems operations. Our expertise in environmental subsurface science has resulted in the Laboratory's emergence as a national leader in mitigating greenhouse gases (GHGs) through geologic sequestration science supporting the Midwest, Southwest, and Big Sky Regional Carbon Sequestration Partnerships, with major roles in the Wallula Carbon Sequestration Demonstration and FutureGen projects. PNNL has more than 191 staff scientists and engineers advancing this capability in the MSL, 331, and Sigma 5 facilities, PSL, Research Technology Laboratory (RTL), and EMSL.

The environmental subsurface science capability provides the basis for PNNL's programs in environmental restoration sciences; fate and transport of subsurface contaminants and legacy waste cleanup; GHG co-sequestration and demonstration; environmental impact assessments for nuclear, geothermal, water/ocean, and wind energy; ecological management; and marine science research. This capability is funded through programs in SC (BER and BES), EM (waste processing, groundwater and soil remediation, nuclear materials disposition), FE (carbon- and co-sequestration), EERE (geothermal technologies, wind and water power technologies), and the U.S. Nuclear Regulatory Commission (NRC) and U.S. Army Corps of Engineers (USACE). This capability advances DOE's missions in scientific discovery and innovation (SC 11, 12, 13, 14, 15), energy security (ES 2, 3, 4, 5, 9, 16), environmental management (EM 2, 3), national security (NNSA 2), and homeland security (HS 3, 7, 11).

3.6 Applied Materials Science and Engineering

PNNL is recognized internationally for its capability in applied materials science and engineering, with domain expertise in materials characterization; materials theory, simulation, design, and synthesis; materials structural and chemical modification; the role of defects in controlling material properties; and materials performance in hostile environments, including the effects of radiation and corrosion. PNNL's strength in this capability is derived from the Laboratory's foundations in chemical, molecular, biological, and subsurface science, and the ability to engineer enabling nano-structured and self-assembled materials, tailored thin films, ceramics, glasses, alloys, composites, and biomolecular materials.

The Laboratory is specifically known for its expertise in radiation effects on materials, solid oxide fuel cells and energy storage materials, solid-state lighting, and organic electronic materials as well as its expertise in developing functionalized nanoporous ceramics for catalytic, sorbent, and sensing applications. PNNL has more than 193 scientists and engineers who contribute to and use state-of-the-art material characterization and imaging instrumentation at EMSL; high- and low-dose radiological facilities, including PSL and the new Physical Sciences Facility (PSF); and laboratories for thin-film material synthesis and deposition, including APEL and RTL.

The applied materials science and engineering capability forms the basis of PNNL's programs in radiation effects in materials; multiscale behavior of structural materials; design and scalable synthesis of materials and chemicals that bridge the mesoscale; fuel cells and energy storage; electric and lightweight vehicle technology; nuclear reactor safety assessment, regulatory criteria, and life extension; and legacy waste forms. It is funded through programs in SC (BES, FES), NE (advanced fuel cycle initiative), EERE (hydrogen storage and fuel cell technology), EM (waste processing), and the NRC. This capability advances DOE's missions in scientific discovery and innovation (SC 7, 8, 9, 10, 18), energy security (ES 2, 11, 13, 14, 15, 16), environmental management (EM 3), national security (NNSA 2), and homeland security (HS 3, 11).

3.7 Applied Nuclear Science and Technology

PNNL is a national leader in applied nuclear science and technology. The depth and breadth of this capability enables PNNL to play pivotal roles in fundamental scientific, nuclear nonproliferation, and nuclear energy efforts. PNNL has domain expertise in ultra-trace detection and analysis, non-destructive evaluation, dosimetry and health physics, international nuclear intelligence analysis, nuclear material security and interdiction systems, fuel cycle characterization, nuclear fuels production and processing, nuclear safety analysis and risk assessment, nuclear detectors, actinide chemistry, online monitoring techniques, and radiochemical process engineering.

PNNL is internationally recognized for our capability in environmental sampling for nonproliferation and nuclear detonation monitoring missions and best known for leadership in developing new science, tools, and techniques for monitoring and predicting materials and process performance for nuclear power applications, performing nuclear safety and risk assessments that include human health exposure impacts, and identifying trace environmental signatures for monitoring nuclear activities. More than 305 staff scientists and engineers support this capability along with uniquely equipped high- and low-dose radiological and ultra-low background counting facilities (PSF), CAT-II radiological chemical processing (RPL), and National Institute of Standards and Technology (NIST) certified calibration (Radiation Calibration Laboratory [RCL]). Additionally, PNNL has outdoor facilities for testing interdiction systems designed for border security as part of the PSF complex.

The applied nuclear science and technology capability forms the basis for PNNL's programs in isotope production, nuclear nonproliferation, tritium target qualifications, health physics, nuclear fuel cycle research and development, radiation portal monitoring, dosimetry, international nuclear intelligence analysis, and weak interaction physics. This capability is funded through programs in NNSA (nonproliferation, defense programs), DHS, NE (fuel cycle), EM (waste processing, nuclear materials disposition), NRC, the Intelligence Community, and SC (Nuclear Physics and High Energy Physics). This capability advances DOE missions of scientific discovery and innovation (SC 21, 22, 23, 26, 29, 30, 31, 32), energy security (ES 2, 16), environmental management (EM 2, 3), national security (NNSA 2), and homeland security (HS 1, 2, 3, 4, 6, 7, 8, 10).

3.8 Advanced Computer Science, Visualization, and Data

PNNL is recognized internationally in advanced computer science, visualization, and data management. PNNL uses its expertise in computing and mathematics to develop scalable analysis

algorithms, high-performance computing tools, data-intensive information systems, and secure computing infrastructures for scientific discovery, predictive modeling, situational awareness, and decision support.

PNNL's unique capabilities and leadership in data-intensive computing applications and architectures is exemplified in three centers. The U.S. Department of Defense (DoD)-funded Center for Adaptive Supercomputing Software-Multi Threaded Architectures conducts research in algorithms, systems software, and programming environments to enable data-intensive applications that do not have spatial or temporal locality and will benefit from novel architectures. Second, PNNL provides international leadership for information analytics through a portfolio of projects support by the DHS and Intelligence Community, which delivers decision-making and analysis tools to intelligence analysts, national and homeland security officials, and first responders and law enforcement personnel. Third, the Electricity Infrastructure Operations Center (EIOC) merges real-time sensor data with advanced computing, bringing together industry software, real-time grid data, and advanced computation into a functional control room for real-time monitoring and management of the nation's electric grid.

PNNL's strengths in data management and informatics support the EMSL and ARM DOE user facilities. PNNL is a leader in computational chemistry, subsurface transport simulation and modeling and simulation for the power grid. For 10 years, PNNL has led the nation in new cyber security capabilities to detect and analyze DOE networks and electricity infrastructure. Leading the DOE Cooperative Protection Program and the Cyber Intelligence Center, PNNL is responsible for the research and development of next generation cyber security sensors, standards for secure communication protocols, design of analytic methods and tools, and operational analysis of the integrity and security of cyber networks. Computer science capabilities include data analysis and visualization, performance and power modeling, programming and execution models, and hardware and software multithreading. Computational math capabilities include upscaling, stochastic partial differential equations, and uncertainty quantification. PNNL has more than 375 staff scientists and engineers supporting this core capability.

This capability underpins PNNL's programs in data-intensive and high-performance computing, scientific and knowledge discovery frameworks, cyber security, information analytics, computational chemistry, computational biology and bioinformatics, and computational subsurface science. This capability is funded through programs in SC (ASCR, BER, BES), Intelligence and Counterterrorism, Electricity Delivery and Energy Reliability (OE), NNSA (nuclear nonproliferation), DHS, DoD, Intelligence Community, NIH, the National Science Foundation, and the U.S. Department of the Treasury. This capability advances DOE's missions of scientific discovery and innovation (SC 1, 2, 3, 4, 5, 6, 12, 13, 14, 16, 26), energy security (ES 10), national security (NNSA 2), and homeland security (HS 1, 2, 3, 4, 5, 6, 7, 8, 10, 12).

3.9 Systems Engineering and Integration

PNNL is an international leader in systems engineering and integration. This core capability focuses on solving complex problems—from concept to deployment—by synthesizing and integrating multiple disciplines and products to develop and implement efficient solutions. The Laboratory defines and interprets complex technical requirements and translates them into fieldable solutions that address economic, social, and engineering considerations. Using a structured approach to understand complex systems throughout their life-cycle, PNNL uses its domain knowledge and experience in engineered systems simulation and modeling; system architecture and design; test, evaluation, and optimization; technology assessment, integration, and deployment; policy assessment and economic evaluation; safeguards and physical security systems; and regulatory analysis, risk assessment, and decision support.

PNNL applies a graded approach to our systems engineering discipline that enables us to deliver solutions in a highly efficient and effective way. PNNL is known worldwide for field-deploying international nuclear materials safeguards, security, and complex radiation detection systems. PNNL also leads in developing integrated building energy technologies, advancing national power grid reliability and

smart grid technology, and conducting large-scale demonstrations of carbon management demonstrations. To support this capability, PNNL has more than 481 staff scientists and engineers and key facilities that include the EIOC, system engineering facility, and Radiation Portal Monitoring Integration Laboratory (part of the PSF complex).

The systems engineering and integration capability is funded through programs in EERE (buildings), EM (waste processing, nuclear materials disposition), OE (infrastructure security and energy restoration), FE (carbon- and co-sequestration), SC (BER), NNSA (nonproliferation), and DHS. This capability advances DOE's missions of scientific discovery and innovation (SC 11, 16, 30), energy security (ES 3, 4, 7, 8, 9, 10, 14, 15, 16), environmental management (EM 2, 3), national security (NNSA 2), and homeland security (HS 1, 2, 3, 5, 6, 9).

3.10 Large-Scale User Facilities/Advanced Instrumentation

PNNL is recognized internationally for its ability to conceive, design, build, operate, and manage world-class scientific user facilities. This capability focuses on the design and development of transformational research tools and techniques that accelerate scientific discovery and technical solutions. PNNL has demonstrated this ability in the design, construction, and operation of the EMSL, DOE's first user facility to deliver a suite of unique and state-of-the-art instruments that accelerate scientific discovery and innovation to advance DOE's missions. This capability also enables PNNL's contribution to the design and operation of the ARM.

EMSL boasts an unparalleled collection of state-of-the-art computational and experimental capabilities that is focused around its three science themes of biological interactions and dynamics; geochemistry and biogeochemistry in terrestrial and subsurface ecosystems; and the science of interfacial phenomena to address critical challenges in DOE's environmental and energy mission areas. Advanced instrumentation is integrated with multidisciplinary teams of users collaborating with expert staff to resolve complex scientific problems. EMSL provides access to instrumentation in high-performance mass spectroscopy, high-resolution microscopy, high-field magnetic resonance spectroscopy and imaging, surface and interface spectroscopies, and high-performance molecular science computing that is unmatched in sensitivity and resolution, sample throughput, and variety of in situ sample environments. The ARM is designed to improve the understanding and representation in climate and earth system models, of clouds and aerosols as well as their interactions and coupling with the Earth's surface. In addition, the G-1 aircraft provides an airborne atmospheric research facility to measure a wide range of aerosol and cloud properties.

Together, EMSL and ARM provide unique opportunities to national and international scientific users to conduct world-class research individually and in collaboration with PNNL staff. Nearly 78 personnel are dedicated to designing, building, operating, and managing large-scale user facilities.

The large-scale user facility and advanced instrumentation capability is funded by SC (BER, BES) and NIH (National Center for Research Resources). This capability advances DOE's missions of scientific discovery and innovation (SC 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 24, 26, 33, 34), energy security (ES 8, 9), environmental management (EM 2, 3), national security (NNSA 2), and homeland security (HS 1, 3).

4.0 Science Strategy for the Future: Major Initiatives

4.1 Scientific Vision

PNNL's scientific vision is to lead discovery in the molecular chemical, biological, and material sciences through the development and use of innovative imaging and analysis techniques, and data-intensive and extreme-scale computing capabilities. This vision will be realized through the success of our seven major initiatives that collectively advance PNNL's leadership in science and technology, and inspire and enable the world to live prosperously, safely, and securely. These seven major initiatives build upon our recognized leadership in our core capabilities (Section 3), strengthen the scientific and technological foundations of the Laboratory, and will result in significant mission impact.

Strengthen U.S. Scientific Foundations for Innovation. Progress in basic science is essential to America's continued prosperity and security in the 21st century. Breakthroughs in fundamental and computational science yield remarkable discoveries and scientific tools that reveal nature's deepest mysteries and advance our understanding of the world around us. They also provide a foundation for delivering science-based solutions in energy, the environment, and national security. Our focus is on the most important scientific challenges—fundamental understanding of chemical and physical processes, understanding global earth system dynamics and impacts, elucidating the dynamics of complex biological and biogeochemical systems, designing and synthesizing functional and structural materials—and the new tools needed to address these challenges.

Increase U.S. Energy Capacity and Reduce Dependence on Imported Oil. America's energy challenges have become more acute and pervasive. There are no simple, immediate solutions. We will continue to rely heavily on carbon-based fuels for another 30–50 years, until renewable sources can scale up to displace them. Growing emissions are propelling long-term earth system changes. And our energy infrastructure is not well-positioned to keep pace with increasing demand. Multi-faceted solutions are needed, and rapid innovation is required. PNNL is focusing on energy innovations aimed at enabling an "energy bridge" that will allow the nation to transition from a carbon-based energy economy to one based on domestic, low-emission resources that are reliable, sustainable, and efficient.

Reduce Environmental Effects of Human Activity and Create Sustainable Systems. The environmental issues that the nation faces are increasingly complex, yet our ability to address them is limited by our scientific understanding and available technological solutions. Our ability to prevent future environmental impacts is limited by the methods available for monitoring and prediction. And, as energy demands increase worldwide, so does the need to balance energy production with stewardship of environmental resources. PNNL will apply its expertise in biogeochemistry, hydrogeology, radiological separations, and process chemistry to solve complex high-level waste issues, and to understand the environmental considerations for siting and monitoring energy facilities.

Prevent and Counter Terrorism and Proliferation of Weapons of Mass Effect. Global terrorism and the threats posed by the proliferation of nuclear materials and weapons will continue to evolve in complexity as adversaries attempt to penetrate our defenses and evade detection. The nation's cyber infrastructure is rapidly becoming the preferred target by international groups who wish to disrupt commerce and pirate intellectual property. Innovative strategies and technologies are essential to counter these dynamic and emerging global threats. PNNL is enhancing America's security by discovering novel threat signatures that enable the nation to better detect, assess, and mitigate new security threats and respond effectively to disruptive events. Our focus is on developing the formalized methods and the analytic framework to systematically construct and validate novel signatures, and on advancing the required measurement and information analytic sciences to enable their detection.

4.2 Major Initiatives

PNNL's seven major initiatives are intended to transform our technical capabilities to achieve our scientific vision. These initiatives are our highest priorities for the next 5–10 years, and are aimed at strengthening PNNL scientific leadership and providing new capabilities to support DOE, NNSA, and DHS missions. Each initiative is described in terms of its vision, outstanding scientific challenges, technical approach, and required resources. These seven initiatives are designed to increase the rate of scientific discovery and innovation and accelerate the deployment of solutions to national challenges.

4.2.1 Controlling Interactions Across Scales to Enable Scalable Synthesis

The Vision. Accelerate the design and deployment of new sustainable and economically viable processes to synthesize materials and chemicals critical to the strategic interests of DOE and the nation. We will transform our understanding of the principles needed to control the assembly of atoms and molecules precisely, rapidly, inexpensively, efficiently (*i.e.*, reducing energy consumption and waste production), and in meaningful quantities. The intended long-term impact is to accelerate manufacturing of fuels and materials that cut the cost of biomass conversion to fuels by half, increase fuel efficiency by 20% through emissions control for lean burn internal combustion engines, decrease the cost of manufacturing multi-ferroic materials by a factor of two, and enable energy storage systems with characteristics of 250 Wh/kg and $100/kW.

Outstanding Scientific Challenges. The interactions and processes controlling scalable synthesis range from the atomic and nano-scales (*e.g.*, at catalytically active sites) to the meso-scale (*e.g.*, interactions controlling three-dimensional self-assembly) to the micro-scale (*e.g.*, microbial interactions controlling energy and matter transfer). The major technical challenge is to understand these interactions and design systems where multiscale interactions and processes function cooperatively. Significant progress has been made by the scientific community to allow us to observe and model processes at atomic and molecular scales. The key to designing complex processes involved in scalable synthesis is an understanding leading to control of meso-scale processes.

Catalytic production of fuels requires processes that selectively make and break multiple chemical bonds, and couple the bond-breaking and making processes with electron transport and transfer to drive energetically unfavorable processes. The primary challenges for these bond-selective transformations are identifying and controlling processes at catalytically active sites; linking processes occurring at multiple sites; and controlling the process environment to facilitate multistep reaction and transport processes.

Emergent energy applications require the design and synthesis of materials with precisely controlled structures on multiple length scales with multifunctional mechanical, electro-optical, or chemical properties that cannot be derived from a single material or a homogeneous mixture of materials. Traditional synthetic processes that use high heat treatment and mechanical or chemical mixing lack the required spatial and structural control. Discovering and designing new materials and molecular assemblies requires controlled atomic and molecular processes to create nano-scale building blocks, and their directed assembly to produce nano-structured materials with mesoscale structure and function.

Biological systems perform complex energy conversions and create unique nano-structured materials with exquisite precision. The primary challenges in predicting the behavior, manipulating, and engineering microbes and microbial communities are to understand how metabolic pathways within individual microorganisms and communities of microorganisms function and can be altered to enhance the production of desired products.

Technical Approach. We adopt the general approach of integrating synthesis, characterization, and theory and computation for studies of model systems to discover the principles underlying scalable synthesis. This approach requires new multi-modal imaging tools that allow interrogation of systems at the molecular scale to characterize the mechanistic pathways of synthetic processes (see the *in situ*

Chemical Imaging and Analysis major initiative). Theory and computation, in particular new multiscale modeling tools and exascale computational capabilities (see the Simulation and Analytics major initiative), will be essential for interpreting the experiments, providing insight into the mechanisms and providing feedback to systematically alter and ultimately control the synthetic processes.

Our approach to designing complex chemical processes uses molecularly tailored active sites to create catalysts with multiple functionalities. The controlled synthesis of nano-clusters on well-characterized surfaces and embedding molecular active sites into nano-structured materials will create molecularly tailored, catalytically active sites and lead to catalysts with multiple functionalities. New high-resolution imaging tools (via the *in situ* Chemical Imaging and Analysis major initiative) to observe reaction processes in operando will probe the influence of catalyst structure, including multiple functionalities, on the specificity and efficiency of the catalytic process. Multiscale modeling tools will bridge reaction events at multiple active sites from the molecular scale to continuum heat and mass transport. Lessons learned from biocatalysts will inform the control of reactant transport and orientation at active sites and will be tested through the reengineering of enzyme catalysts. PNNL's Center for Molecular Electrocatalysis (an Energy Frontier Research Center) has demonstrated that principles learned from enzymes could be used to create an inorganic catalyst that is 10 times faster than the enzyme in producing hydrogen gas. This work was reported in the August 12, 2011 issue of *Science*.

Our approach to designing new materials and molecular assemblies uses "bottom-up" synthesis methods to produce materials with controlled mesoscale structure and function. We will understand fundamental, governing principles that direct the formation of zeolites; metal-organic framework structures; nano-porous and nano-crystalline materials widely studied for catalysis; energy storage materials; and carbon capture materials. Bottoms-up methods use molecular ligands to control interfacial nucleation and growth processes that direct nano-structure formation and self-assembly. The precise control of nucleation and self-assembly on two-dimensional templates, combined with spectroscopic probes of interfacial structure and processes, and multiscale simulations will provide insight into the energetics of structural rearrangements. The fundamental understanding of molecular assembly at surfaces and metal oxide growth on uniform and patterned templates gained from these studies will be extended to the synthesis of more complex, three-dimensional nano-structures for energy applications. We will develop methods that deploy biomolecular assembly methods to create next-generation bio-composite materials, which draw upon bio-assembly techniques to control overall physical properties and facilitate the incorporation of disparate functional proteins. Research at PNNL demonstrated the ability to synthesize titanium oxide and graphene nanostructures that greatly improve the performance of lithium-ion batteries. Vorbeck Materials, a startup company using this discovery to improve the performance of lithium-ion batteries, was named by Energy Secretary Steven Chu as one of three winners of "America's Next Top Energy Innovator" challenge in 2012.

Our approach to predicting the behavior, manipulating, and engineering microbes and microbial communities is to create sets of integrated technologies that lead to a mechanistic and predictive understanding of biological systems. Advanced multiscale *in situ* imaging tools for characterizing structure and function under operating conditions and new multiscale modeling approaches are critical to this effort. They will be used to create unique microscale environments, integrate 'omics data from microbial communities and their members, interrogate metabolism and kinetics using stable isotope analysis, and develop mathematical models to analyze the micro-scale biological processes and predict their macroscale effects. This will allow us to interrogate, model, manipulate, and engineer metabolic pathways using system-level and synthetic biology approaches in natural and constructed microbial systems. Our concept for biological systems engineering involves platforms beyond those used traditionally for metabolic engineering and synthetic biology. To take advantage of alternative engineering platforms and to bypass the need for teams of researchers to invest years into developing genetic systems, we need more robust means for the optimization of existing and the design of novel reaction processes or pathways and cellular functions through genetic and metabolic engineering. Work at

PNNL has shown how fungal systems can be designed to synthesize large quantities of desired enzymes. This capability was recently enlisted into the Joint BioEnergy Institute to make fungal-enzyme cocktails for biomass deconstruction.

Required Resources. This major initiative builds on our leadership of the Institute for Integrated Catalysis and strong programs from BES (Catalysis; Solar Photochemistry; Chemical Physics; Geosciences; and Materials Discovery, Design, and Synthesis); the Center for Molecular Electrocatalysis; and EERE, OE, and FE programs. The microbial communities work builds on leadership roles in the BER Genomic Sciences and Subsurface Biogeochemistry Research Program and EERE biomass programs. Materials synthesis efforts build on BES programs in materials synthesis and strong EERE, OE, and FE programs in energy storage and carbon capture. Laboratory Directed Research and Development (LDRD) investments are building new capabilities in nano-structured catalyst design and synthesis, scalable materials synthesis, and control of microbial systems. Theory and computation is a cross-cutting capability required for this major initiative. The development of new algorithms and tools, particularly multiscale modeling capabilities, and their implementation on leadership-class computing architectures will benefit from our programs from ASCR.

Laboratories with environmentally controlled space for imaging tools and a high density of fume hoods to support synthesis are critical and proposed in the new Chemical Sciences and Imaging Laboratory (CSIL; Section 4.3), which will enable co-location of capabilities in catalysis science; molecular science; materials discovery, design and synthesis; and the Center for Molecular Electrocatalysis. Access to unique characterization tools in EMSL, and micro-engineering and micro-analytics capabilities to design and sample unique microscale environments, are also required.

The addition of senior leadership is needed in several areas to help develop and execute the vision of this major initiative. These include leaders in microbial systems bioengineering, catalyst materials synthesis, theory and computation for multiscale modeling, biomaterials design and synthesis, and polymer chemistry and solid-state physics. Strong partnerships are in place with WSU, the University of Delaware, and the Catalysis Research Institute at the Technische Universität Munchën in catalysis. Partnerships have been developed with Argonne National Laboratory (ANL), Lawrence Berkeley National Laboratory (LBNL), and Sandia National Laboratory (SNL) in the materials synthesis and energy storage areas. Partnerships in microbiology include the University of Washington (UW), University of California Berkeley, Montana State University, Pennsylvania State University, University of Minnesota, and University of Wisconsin. New programmatic funding is needed to sustain this work. Significant investment in laboratory infrastructure is needed to provide modern chemical synthesis and materials characterization laboratories.

4.2.2 Efficient and Secure Electricity Management from Generation to End Use

The Vision. Integrate data from new sensor technologies with communication networks, ultralow latency data management systems, high-performance computing, and decision analysis capabilities to enable real-time monitoring and operation of the U.S. electric grid. PNNL will deliver new analytic methods and models that enable high fidelity simulation of the power system from generation to end-use and over very wide geographic areas; develop HPC-compatible software architectures that ensure that these rapid convergence of these new simulations (solving in microseconds instead of minutes or minutes instead of days); and develop visual analytics that allow operators to respond more effectively to grid disturbances. These developments will deliver unprecedented system reliability, resiliency and efficiency while also enabling new load demands (*e.g.*, large numbers of electric vehicles) and significant amounts of intermittent and variable generation (*e.g.*, wind, solar).

Outstanding Scientific Challenges. Within 3–5 years, new devices such as phasor measurement units, distribution automation systems and smart meters will provide the data necessary for transmission and distribution operators to monitor, assess, understand, and respond to grid performance in real time

across a wide area and under emerging contingency situations, resulting in unparalleled system performance. Three transformations are needed to achieve this performance.

Transform Grid Operations and Management. The first challenge is to develop a diverse interconnection-scale network to collect and transfer large volumes (tera- to petabytes) of data at widely varying rates (several thousand samples per second to one sample every few seconds). This new "data highway" requires advanced protocols, methods, and software for secure routing across wide geographic areas at transfer rates not currently possible. New data integrity requirements must be developed and the infrastructure must be able to respond quickly to changing conditions and data requirements. The second challenge is to develop methods to analyze the incoming data stream, creating the means for real-time monitoring of the grid condition, predicting the grid's future state, assessing potential contingencies for perturbation response, and evaluating potential control responses. Today's tools provide a retrospective view of grid performance with a limited set of contingency analyses. The third challenge is to translate the data and analytic information into a signal that grid operators can understand and act upon. Data are generated at micro-second intervals and operators make decisions in near-real-time, meaning new decision support tools must be developed, tested, and deployed.

Transform Demand Management. Today's grid allows no interaction between supply and demand making large-scale improvements in the efficient end-use of power difficult. Transforming demand management requires models to translate real-time system dynamics into control systems that consumers – or their appliances through SmartGrid technology – can act upon. In return, models are needed to aggregate load information and translate that information into signals that grid operators can use to effectively and efficiently manage and operate the grid.

Transform our Ability to Address Advanced Persistent Cyber Threats. System-wide interoperability and security standards are central to our ability to protect the grid infrastructure and associated data streams from advanced, persistent cyber-threats. In addition, advanced cyber-analytics that enable threat prediction and response across the entire continental system must be developed, tested, and deployed.

Technical Approach. This initiative involves three technical thrusts:

Advanced Sensor Network Architecture and Real-Time Data Management. Working with regulatory and standards bodies to define and develop network architecture and interoperability standards, we will advance network design, the real-time management of massive data sets, visual data analytics, and cyber security techniques for rapid, secure, high-fidelity delivery of large data sets. We will develop advanced algorithms and software to detect and predict network failure or compromise and dynamically identify, filter, and reduce data based on conditions and locations. To understand traffic behavior under congestion or failure conditions, we need large-scale sensor network simulation models (>1 M nodes) requiring massively-parallel high-performance computing power. Output from these models will allow the evaluation of network efficiency and existing data network protocols. By developing new routing protocols that support richly connected mesh network topologies and enable multipath routing in wired and wireless networks, we will support data traffic balancing across a richly connected network to increase efficiency and reliability. Central to this is a focus on cyber security measures for routing protocols to prevent traffic diversion and denial of service attacks. Our focus will be to create a reliable, cryptographically secure, and easy-to-use identity and key management protocol stack for enrolling, managing, and removing millions of grid devices, leveraging major initiatives in Signature Discovery and Exploitation for Threat Detection and Reduction and Simulation and Analytics. PNNL recently completed the PowerNET laboratory which provides the ability to simulate various networking architectures and to test device interoperability and data security in a real-world environment.

Analytic Methods for Real-Time Monitoring, Operation Management, and Control. PNNL will lead the development of real-time, wide-area models, simulation, and analysis methods and tools that will transform interconnection-scale grid operations. Advanced filtering, optimization, and statistical

techniques for deriving and validating dynamic grid models from measurement data will be developed, along with next-generation grid models using new scalable parallel algorithms and high-performance computers capable of real-time execution. This effort requires the development of operating systems and runtime and communication layers, as well as computational performance analysis, optimization, and modeling for real-time applications running on high-performance computing platforms. To advance real-time contingency analysis, mathematical approaches that, when combined with high-performance computing, will effectively converge on solution sets that predict multicomponent failures are needed. Using PNNL's expertise in data and meta-data management, research efforts will also explore software systems to organize and transfer data from large complex data sets into real-time models and simulations.

Visual Analytics and Real-Time Decision Support. Using PNNL's EIOC and the capabilities developed in the PNNL-led National Visualization and Analytics Center, a comprehensive, versatile visual analytics tool suite specifically designed for the grid will enable consistent information exchange, improve situational awareness, and allow power grid planners and operators to react quickly and effectively to emergency situations. These efforts will build on advances in human factors and cognitive science as applied to the behavior of planners and operators. Combined with high-performance computing techniques, graph analytics will explore the cause-effect relationship between both potential failures and consequences and remedial actions and effects to support real-time decisions. For comprehensive situational awareness, new visual tools and methods must be developed for the grid that allow multiple visualization interfaces to interoperate over the same data streams in a coordinated way. This requires standards and protocols for linking grid modeling and visualization toolkits, along with new visual metaphors to represent grid behavior across temporal and spatial scales. Probabilistic models to assess potential outcomes of operational decisions and linked statistical and visual representations of uncertainty in both raw sensor measurement and derived data will communicate the potential consequences of alternate decisions. Decision support technologies with new mathematical and statistical models of human decision-making processes and grid operator behavior will be developed. Coupled with ontological representations of grid domain concepts, these models enable automated reasoning agents to identify and mitigate human bias and error. The tools that human operators use will be instrumented to collect real-time data on operator actions, and when coupled with incoming sensors streams, use machine learning techniques to suggest potential courses of action based on current conditions. Algorithms that compare operator actions against decision templates will identify potential errors and emerging conditions of which the operator appears unaware. Significant early progress in this area includes development of a new contingency analysis package that leverages parallelization to deliver extraordinary solution times and present results through a new graphical display that is currently being evaluated by control room operators. PNNL also demonstrated dramatically faster HPC versions of the State Estimation and Financial Transmission Rights software tools that deliver results in time spans much more compatible with real-time grid operation. Demonstration of these tools was enabled in large part by the PNNL institutional computing (PIC) investment.

Required Resources. This initiative builds on PNNL programmatic leadership in advanced grid reliability, demand response, and smart grid technologies. LDRD investments will enhance capabilities in sensor network and data management; computation, analytics, and simulation; control paradigms; and visualization and decision support, including strategic hires in power systems analysis, high-performance computing, and network design. The most important new resource is a facility that expands upon capability resident in the EIOC to provide a new capability and capacity to engage other researchers (DOE laboratories and academia), the vendor community, and system operators to demonstrate the power of the new simulations and decision support systems developed by PNNL (see Section 4.3). In addition, this facility will provide laboratories for evaluation of communication/control/computing network architectures and new power electronics technology, exploring key issues such as data transfer latency, interoperability and security. Together, these new laboratory spaces will position PNNL as the national

grid R&D center with the ability to demonstrate the power of new sensor data and new models to enable real-time grid visualization at the interconnection scale.

4.2.3 Coupling Earth and Energy Systems for Sustainability

The Vision. Develop a modeling system that allows the exploration of meaningful and implementable strategies that sustainably balance national energy needs and security with natural resources management.

Outstanding Scientific Challenges. Our focus is on the interactions among the Earth and energy systems, human activities that influence these systems (*e.g.*, energy production and use, agriculture, land use change), and other natural systems (*e.g.*, ecosystems, biogeochemical cycles, water cycle) that are integrally linked to both. Developing an integrated and dynamic systems understanding of Earth and energy systems requires us to meet these critical scientific challenges, and will require cross-disciplinary research across modeling, experimental and observational science, and engineering communities.

Understanding and Modeling Key Driving Forces, Processes, and Feedbacks. Accurate assessments and predictions of Earth systems and Earth system-changes require a detailed understanding of the fundamental driving forces, the key process-level mechanisms and feedbacks that influence the rate and magnitude of changes in Earth systems, and how the Earth system interacts with human activities. Progress in these areas depends critically on detailed long-term observations, targeted laboratory experiments and field campaigns, and integrated models capable of resolving the key feedback processes among coupled Earth-energy systems on decadal to centennial time scales and across regional to global spatial scales. Data availability will be a critical challenge for both model initial condition and parameterization as well as evaluation strategies.

Identifying Key Systems Vulnerabilities and Impacts. To understand the potential impacts of human-induced changes in Earth systems, we must understand the vulnerabilities of natural and human systems (*e.g.*, energy infrastructure) at the regional scales where impacts are often felt most acutely and where climate-related decisions are typically made. For example, understanding how Earth system changes influence the competition for land, water, and other natural resources will enable us to define the observations, experiments, and modeling strategies needed to improve assessments of the vulnerabilities in these systems. We must also understand and anticipate the tipping points that exist in human or natural systems that endanger the sustained provision of energy and ecosystem services.

Analyze and Evaluate Response Options and Decisions. Responding effectively to changes in Earth or energy systems requires identifying and addressing key sources of uncertainty, improving the accuracy and reliability of integrated models, and developing tools capable of providing targeted information for the scientific community and decision-makers. Once uncertainties are appropriately characterized and quantified, the ramifications of different response options and decisions can be understood and communicated. This information can also be used to guide future research directions.

Computational Resources and Engineering. Developing an integrated framework that dynamically links human activities (*e.g.*, land use, energy demand) with physical (*e.g.*, climate) processes and subsequent analyses will require high performance computing with new approaches in software engineering and architecture development. Communication and feedbacks between the model components will have to account for variable time steps, spatial scales, and software platforms.

Technical Approach. Our technical approach is described in the following six research thrust areas:

Improved Energy Systems Modeling with Transportation. There is an urgent need for tools to model complex energy systems and their interactions with natural systems across a timescale that is relevant for infrastructure investment (50 years). We recognize the need for improved policy analysis, risk assessment, and infrastructure planning tools for building out national energy infrastructure for meeting the needs of the U.S. and global economy in the 21st century.

Oak Ridge National Laboratory (ORNL) and the Electronic Industries Alliance (EIA) have developed sophisticated technology choice and transportation service demand models (*e.g.*, how many vehicle miles traveled as a function of economic activities and disposable income). EIA has developed TRAN, a transportation sector model that currently resides in and is operational at PNNL. We will modify TRAN, and link to actual infrastructure (roads, railroads, water ways, and airports) through the Center for Transportation Analysis (CTA) infrastructure available from ORNL. Coupling the transportation sector model with infrastructure will enable unanswered questions to be addressed regarding infrastructure constraints that limit the growth of transportation services. For example, the greater Seattle area can no longer expand because of interstate limitation. If Washington state's population grows 50% by 2050, the transportation needs for this increase and the associated growth in the State's economy cannot be met. More importantly, no current modeling framework can address this challenge. Coupling TRAN to CTA's actual road routing model will enable the development of scenarios to potentially remedy this situation.

Integrated Observations, Analyses, and Assessments. PNNL has made many contributions to the knowledge base that underpins climate and global change research—*e.g.*, researchers at the Joint Global Change Research Institute (JGCRI) published an analysis showing that worldwide sulfur emissions, after declining for a decade, rose again from 2005-2010 due largely to international shipping and the growth of the Chinese economy. The Laboratory also manages the ARM program, and PNNL scientists regularly contribute to national and international climate and global change assessment reports. Developing the observational and analytical capabilities to support the development, analysis, and evaluation of adaptation and mitigation efforts is as important as understanding the underlying chemical and physical processes driving climate change. Key to this research thrust is identifying where insights are most needed and developing the appropriate approaches for delivering information, including insights on human behavior and decision-making. Macroeconomic models typically assume that humans make decisions consistent with traditional economic theory. Complex, multi-attribute choice models are employed at the microeconomic level, while behavioral psychology and game theory research explore irrational decision-making. Several PNNL programs are exploring human decision-making and motivations. Bringing game theory and decision analysis expertise into the integrated assessment framework allows the evaluation of model sensitivities and enables the development of alternative representations of human behavior.

Integrated Models of Earth and Energy Systems at Global and Regional Scales. PNNL develops and contributes to models capable of simulating the complex interactions among climate, energy, and human activities. The iRESM provides an integrated modeling framework to address regional Earth-energy system interactions (*e.g.*, how energy production influences regional climate and how that, in turn, constrains land and water use). PNNL also plays a leadership role in developing integrated global Earth system models and develops and applies world-class integrated assessment models. Careful design of these modeling frameworks facilitates numerical experiments to improve understanding of nonlinear, composite system behaviors, including system feedbacks, scaling properties and characterization of uncertainties in both individual model components and the overall framework. Establishing a robust evaluation process using test beds ensures model evaluation will increase understanding, quantify uncertainties, and lead to model improvement. Models can be evaluated by comparing model simulations with observations, analyzing model sensitivity to parameterizations and external forcings, examining sources of model bias, and inter-model comparisons. The test beds require multiple geospatial datasets including climate, hydrology and water use; land cover and land use; water resource management, energy, and transportation infrastructure for the regions of interest. The importance of understanding global challenges at a regional level is highlighted in an upcoming publication, "The Regional Nature of Global Challenges: A Need and Strategy for Integrated Regional Modeling."

Integrated Understanding of Water. PNNL strengths include atmospheric measurements and modeling (*e.g.*, water vapor, clouds, and precipitation), surface and groundwater hydrology, biosphere and ecosystem interactions, coastal modeling, and water-energy interactions and modeling. We have

ongoing collaborations with several universities and other national laboratories (UW, USACE, ANL, SNL, ORNL) with relevant expertise as well as existing programs (EERE, Coast Guard, DoD). Our focus is on modeling water management infrastructure and linking atmospheric, terrestrial, and coastal processes; biosphere and biogeochemical modeling (including dynamic vegetation modeling); multiscale modeling of the water cycle; and access and utilization of remote sensing data. PNNL scientists have, for example, made important improvements to the hydrology and river routing modules in the Community Land Model as well as a new uncertainty quantification framework. In addition, allocation of water demand either through water markets or an *a priori* hierarchy will be developed within iRESM to account for possible conflicts of water for agricultural and energy production.

Developing a New Capability that Links Upland Land Systems to Coastal to Marine. An outstanding scientific gap is in understanding how nutrients are processed from agricultural systems downstream to coastal zones. In addition, there are limited capabilities for quantifying the vulnerabilities of energy systems to changing climate. PNNL has expertise in physical ocean and coastal modeling, as well as sophisticated observatories in Seattle and Sequim. This expertise has already been applied, for example, to better understand the impact of sediment transport on hurricane formation in the Atlantic. We will utilize our capabilities and develop a biogeochemistry component that will enable understanding the magnitude and rate of nutrient and sediment transport from upland systems to coastal systems. In addition, by linking to a regional ocean modeling system we can demonstrate how nutrients are processed in coastal systems through their residence times and eventual deposition. Understanding and quantifying vulnerability of energy systems in coastal zones is critical for future siting of thermo-electric, as well as existing oil and gas infrastructure.

Improved Tools for Understanding Uncertainty and Managing Data. Central to climate change research is characterizing and reducing uncertainties surrounding model projections. PNNL scientists have a long history of contributing to the characterization and quantification of sources of uncertainty for climate change assessments, and have recently developed a framework for evaluating uncertainty in integrated models. Sources of uncertainty include observational data sets, model performance, and needs of decision-makers and other stakeholders making adaptation and mitigation decisions. As described in a forthcoming paper in *Mitigation and Adaptation Strategies for Global Change*, these communities will be engaged to understand decision making needs with respect to uncertainty. Building on this understanding, methods and tools will be developed to support decision-making in the face of risk and uncertainty in climate change impacts and provide confidence that the science is robust and able to support decisions. Data management is a critical activity that underpins virtually all aspects of climate and Earth system science, including the research thrusts identified above. Visualization and other tools for providing these data to both researchers and decision makers is an equally cross-cutting and important challenge and we are working to develop these tools and methods through other PNNL major initiatives.

Required Resources. PNNL will draw on existing programmatic leadership in climate change science. Increased programmatic support for scientific leadership in measurement and data analytics, integrated assessment, climate modeling, biogeochemistry and environmental microbiology, and computational science and program management is needed, as is the continuation of current LDRD investments. The PIC program is important for access to mid-range computers for process model development and testing. Access to high-performance computing facilities (up to and including exascale), data manipulation tools that facilitate data extraction, visualization, and manipulation, and peta-scale data storage is also required. Strategic partnerships with the UW, University of Maryland, and the National Center for Atmospheric Research as well as ORNL and SNL are also envisioned.

4.2.4 Signature Discovery and Exploitation for Threat Detection and Reduction

The Vision. Predict, detect, and mitigate increasingly dangerous and complex threats to global security and our nation's critical infrastructure by merging measurement sciences with powerful

computational and data analytics architectures to discover novel signatures and drive technical advances in how threat signatures are collected and analyzed. These new tools, methods, and architectures will be initially aimed at hindering nuclear trafficking and strengthening nonproliferation, enabling enterprise-scale dynamic operation, automated defense and resiliency in our critical cyber infrastructure, and informing the optimal response to extrinsic health threats from a pandemic or biological-agent attack.

Outstanding Scientific Challenges. Traditional threat detection and mitigation relies heavily on the measurement of a signature that correlates with the phenomenon of interest. The process by which signatures are identified and/or constructed is generally *ad hoc*, highly domain specific and often subject-matter-expert driven. Our aim is to establish broadly applicable methods and analytical frameworks that integrate expert-driven and data-driven elements to better detect and understand complex threats that straddle multiple measurement domains and signature types. For an integrated, systematic approach to signature-based threat detection and analysis, the major science and technology challenges in measuring signature quality and stability, and validating its utility require new algorithms and methods for applying expert judgment to processes for abstracting information from massive amounts of multisource heterogeneous data, fusing the abstracted information along common feature vectors, and applying formalized methods for exploring the information to uncover new complex patterns and relationships. Discovering novel signatures and using them to analyze threats will both be aided by and create the demand for new collections and measurement systems. Major scientific challenges also exist due to the current limitations on our ability to detect very weak or rare signals in the presence of a high natural background or noisy environment, or one where intentional obfuscation and active deception are present.

Signature Construction and Validation. No formal methodology exists for defining, constructing, and testing signatures. The development of signatures for increasingly complex threats is a challenge because features of interest lie at knowledge domain interfaces. Signatures may be derived from primary indicators, but secondary and tertiary effects also warrant attention. Methods that couple language- or communication-based analysis (text, social media) to technical data (measurements, image analysis) in a meaningful data analytics context are nascent. Signature quality varies widely depending on data set completeness and background noise. There are limits to what can currently be achieved using sparse data in a noisy background. Advanced mathematical and statistical algorithms need to be developed to understand the value of a composite signature versus the sum of its individual contributions.

Signature Dynamics and Detection. Signatures can change over time due to fluctuations in background conditions, intentional obfuscation, or temporal changes in the threat. Near real-time signature monitoring will allow tracking of temporal effects and commensurate revisions to exploitation schemes. The mathematical and scientific underpinning of signature dynamics is a key gap. Signature detection on large data sets is typically performed in “forensics” mode. No tools exist for near real-time analytics based on streaming sensor data. Multi-source data integration and near real-time analytics are notable gaps that, if filled, could facilitate a major transformation in decision support. Another challenging area is rapid image analysis, where tools are needed for rapid processing of video and other multi-modal, multi-dimensional data sets for stand-off threat detection. There is an effort underway that applies bioinformatics-inspired methodologies to discover signatures or to monitor signature drift that occurs as a consequence of changes to the underlying target phenomenon. Major achievements to date include the development of automated methods for identifying and grouping similar features within a dataset and then representing them with an alphabetical character. In this way, complex data sets can be transformed into simple, linear, alphabetical sequences, and powerful inexact matching capabilities ordinarily used to search for genetic markers can now be used to detect and redefine evolving signatures.

Technical Collection and Measurement Science. At ultra-trace concentrations, physical, chemical, biological (and cyber) phenomena and associated signatures are dominated by rare events, and surface and nano-scale behaviors become increasingly important. Surface-dominated interactions can alter signature species and impact sample collection and measurement. Understanding the environmental

science of ultra-trace signatures and its impact on collection and measurement are major challenges. Reducing detection limits for measurement techniques by orders of magnitude allow more options for detecting and mitigating threats. Greater sensitivity and precision allow higher confidence, less sampling, and the potential to field advanced technology for mission support monitoring. Multi-modal, orthogonal techniques that take advantage of disparate measurements for diagnostics, prognostics, and forensics are needed. Efficient and selective separations coupled to high sensitivity analytical instrumentation could yield breakthroughs that would transform signature detection and exploitation.

Signatures for Living Systems. Biological systems can perform separations from complex mixtures with high specificity, and the exposure history can impart unique markers and affect metabolism. The signatures of such phenomena in the science of the "exposome" are emerging. Understanding how living system respond to trace materials will provide additional techniques for signatures detection and exploitation. Decoupling the exposure-based signatures from those dictated by the genome is particularly challenging, and detection limits are poorly understood. Again, multi-modal techniques such as integrated 'omics will provide the best opportunity to make advances.

Technical Approach. PNNL has long-standing externally funded programs in nuclear nonproliferation signatures discovery and exploitation and developing and deploying new ultra-trace measurement techniques for national and homeland security. We also have notable capability and ongoing programs in chemical and biological forensics, disease prediction, subsurface science, climate change science, and critical infrastructure protection.

A critical capability that underpins this major initiative is information analytics where PNNL maintains active research and development efforts with a multitude of clients in the homeland security, defense, and intelligence community. The direction of this research is continuing to evolve from its historical base of visual analytics to support unstructured text analysis and a future dominated by increasingly large and distributed data sources that demand new scalable heterogeneous multisource analysis and fusion technologies. Our technical approach involves merging measurement sciences with powerful computational and data analytics architectures to advance the scientific foundation of signature construction, validation, detection, and exploitation and deliver unprecedented prognostics, diagnostics, and forensics capabilities for the nation.

Signature Construction and Validation. Human- and machine-based approaches will be coupled to develop a robust and reproducible protocol-based process for signature composition. Human approaches, focused on identifying relevant signature features from multiple domains, will be coupled to conceptual models to extract key parameters and features for use in signatures construction. In parallel, we will build upon existing expertise in analytics and algorithm development to explore clustering and pattern recognition modalities as a substitute for subject-matter-expert-driven signature construction. These two approaches offer a robust and defined process for signature assembly and identification. Validation of the signature requires understanding the statistical confidence with which the signature can be used for indication or prediction. Statistical methods will be developed to appraise the significance and correlation factors of anomalies from data sets. In addition, econometric techniques help us understand cost-benefit tradeoffs in signature collection, allowing the relative valuation of each composite signature dimension. In FY 2011, an internal investment in signature discovery was started to develop the systematic process and set of advanced analytic tools aimed at accelerating the discovery of new signatures in any domain. This effort has produced a generalized methodology for formalized signature discovery, number of conference papers and manuscripts for publication, sponsored guest speaker seminars, and actively recruited several new technical staff to PNNL ranging from entry level PhDs to senior researchers, including the Chief Scientist for the investment.

Signature Dynamics and Detection. Inexact matching algorithms will be extended to provide tools for tracking temporal changes in signatures, enabling an understanding of signature shelf life and provide a quantitative basis for the time value of a signature. Change detection algorithms will be developed to

understand whether new signatures can be automatically updated or augmented to allow signature tracking over a larger dynamic range. Signature profiles (*e.g.*, time-series fingerprints comprising multiple biomarkers for exposure identification or temporal changes in the isotopic composition of a sample during radioactive decay) will be used to create time-dependents to support algorithm development. Detection will focus on the challenges of large data sets, incomplete or corrupted data sets, and extraction of signatures from noisy backgrounds. Data intensive computing techniques will be applied to optimize data triage in the presence of confounding noise. Re-sampling and Bayesian techniques will be used to reconstruct data incomplete data sets, and new techniques such as compressive sensing will also be explored. One of the research areas within the signatures investment is aimed at developing a statistical network model for integrating various types of data sources using a Bayesian network to produce a composite signature that is associated with various research institutions or laboratories. This model could be used, for example, to help identify an institutional specific signature for the forensic analysis of a bioagent release. The structure of this model has been designed and coded for initial testing. A manuscript is under development that describes the model efforts to date.

Technical Collection and Measurement Science. Integrating measurement sciences with applied mathematics and statistical algorithms will accelerate theR&D life-cycle and shorten the time from signature discovery to exploitation. World-class analytical instrumentation will continue to be developed where novel separations approaches allow the use of ultra-trace signatures. Next-generation threat detection systems will move toward multi-modal detection and be capable of real-time modification as threats progress, allowing adaptation of detection and decision-making. We will capitalize on advances in low-power computing platforms and architectures that embed analytics directly onto sensor platforms, enabling on-board data processing to overcome “large data” limitations in fielded systems, and our expertise in exposure-based signatures will be used to understand their practical limits and exploit them in practice. Another area of active research involves applying the methods of compressive sensing to infrared spectroscopy measurements that are employed to detect the composition or presence of selected chemical compounds in air at extremely low concentrations or in the presence of interfering species. The goal of this work is to develop a generalizable analytic method that can identify and accurately reconstruct a full observation from a partial sampling or a low resolution data set across a broad range of measurements.

Resource Requirements. Strategic hires in mathematics, statistics, and data analysis with backgrounds in physical sciences are required. In addition, the PIC program is an important resource for providing mid-range clusters with significant data storage and movement capabilities needed to perform experiments and collaboratively visualize results. The modernization of PNNL’s systems engineering and integration capabilities as described in the 10-year facilities and infrastructure plan is also essential to developing the next generation of detection systems that exploit newly discovered signatures.

4.2.5 *In Situ* Chemical Imaging and Analysis

The Vision. Create a suite of integrated, *in situ* chemical imaging and analysis capabilities to accelerate understanding, design, and control of molecular, biological, environmental, and multi-component materials systems. This initiative will transform the way we do science and establish PNNL as a leader in the development of multi-modal integrative imaging tools.

Outstanding Scientific Challenges. Critical challenges exist in four major areas:

Systems Biology and Microbial Communities. Chemical imaging at the spatial resolution of the microenvironment (< 50 microns) for multiple chemicals as well as cellular macromolecules, and analyses that can extend below the single microbe and are capable of data mining large, complex sets of macromolecule sequences and their associated environmental metadata will substantially accelerate our understanding of microbial communities. Key challenges are development of experimental platforms for imaging microbial communities, and the development of analytical techniques and probes to provide

multi-modal information of cellular machinery. Of particular importance are the capacities to analyze fluxes of chemical components and determine how cells dynamically alter their microenvironment.

Chemistry and Materials Science. Advances in scalable synthesis, catalysis, radiation stability, sensor development, corrosion, and defect-induced property modification rely on correlations between resident structure and chemistry, and exploiting those correlations to control the assembly of structures with targeted behavior. Integrating chemical spectroscopic probes and structural imaging instrumentation with increasingly higher spatial and temporal resolution, and visualizing transient local field variations manifested by stress, dielectric constant, or temperature that collectively contribute to extensive materials properties will accelerate our ability to scalably synthesize mesoscale materials and chemicals with the desired properties. The resulting massive data sets will require sophisticated image interpretation approaches and trend identification algorithms for real-time analysis. *In situ* and non-destructive measurements, particularly for solution self-assembly processes and the analysis of buried interfaces, are critical to improving membrane performance and designing innovative chemically active structures for new catalytic materials, battery electrodes and solid-state electrolytes, and robust sequestration materials.

Energy and the Environment. The development of efficient and selective catalysts for alternative fuels and emission control, breakthrough materials and technologies for large-scale energy storage, low-cost carbon capture and sequestration materials, nuclear materials and spent fuels, subsurface science and marine technologies will all benefit from new chemical imaging and analysis tools. Understanding the structures and properties of these materials and chemicals under static and dynamic conditions requires imaging and analyzing at relevant temperatures and pressures representing realistic operating conditions.

National and Homeland Security. The detection and characterization of chemical, biological, radiological, nuclear, or explosive (CBRNE) threats involve spatial scales ranging from wide-area surveys to the microscopic. New chemical imaging and analysis tools can guide sampling, provide primary threat screening, and cue additional analysis. For particulates, knowledge of the chemical distribution can provide insight into the history, formation processes, and environmental interactions of the sample. Samples often undergo several individual measurements, which are “merged” post-processing, and the sample registration and merging processes can be very challenging. The development of tools for the acquisition of simultaneous, multi-dimensional data will accelerate analyses and improve confidence in the results. Security challenges are typically focused on the “needle in a haystack” scenario, looking for rare events and thus need both imaging and analysis tools aimed at rapid analysis and prioritization.

Technical Approach. Our technical approach is focused in four areas:

Developing Light-Source-Based Probes for Three-Dimensional Tomographic Imaging and Structural and Element-Specific Interrogation. Chemical analysis and identification through direct imaging is a powerful tool for atomistic understanding and light-source capabilities with nanometer-scale resolution, element specificity, and trace element analysis will allow researchers to go from model system observation to real-world molecular manipulation. State-of-the-art main light-source-imaging capabilities include x-ray tomography, scanning transmission x-ray microscopy (STXM), inelastic scattering imaging, and coherent diffractive imaging. One example of the power of this multi-modal approach is that the three-dimensional information of a biological cell can be imaged using x-ray tomography with a spatial resolution of about 50 nm. Imaging the cell components with high-resolution electron microscopy, and combining and correlating these results, leads to a complete atoms-to-microns picture of the cell. Elemental and chemical-state-specific STXM capability has lateral resolution of approximately 20 nm at light sources, providing information about the material’s electronic structure. A cryo-tomography capability with 20-nm resolution in STXM could be an alternate option for the x-ray tomography. STXM and inelastic x-ray-scattering tools can also be used for *in situ* measurements, and the result correlated to laboratory-based *in situ* electron- and optical-microscopy measurements. Maintaining sample registry between systems is critical, and new sample stages and controlling software need to be developed. X-ray Tomographs of *Schewanella* biofilms were taken at the Advanced Photon Source and revealed that our

cryo-tomography protocol is suitable for full field imaging of multiple microbes buried in the extracellular polymeric substance. This work is being presented at an invited talk at the APS user meeting and is being prepared for publication.

Combining Optical, Electron, Ion, Mass, and Scanned Probe Microscopies to Understand Chemical and Biological Mechanisms. Atomic-level imaging and spectroscopic analysis of materials under *in situ/operando* conditions can be done by extending the state-of-the-art aberration-corrected scanning transmission electron microscopy/TEM and other complementary microscopy and spectroscopic imaging capabilities. New capabilities will be developed to enable complementary integration of site-specific atomic resolution structural and chemical information, including scanning transmission electron microscopy/TEM, atom probe tomography, and focused ion beam and scanning electron microscope. We also will develop mass spectrometry (MS) imaging capability and combined with secondary-ion-mass-spectrometry and cryo-electron microscopy capabilities image at length scales ranging from microns to nanometers. Combining the atomic force microscopy with optical capabilities such as tip-enhanced (infrared) imaging is also planned. MS imaging offers high sensitivity, speed, and chemical specificity, enabling simultaneous identification of various classes of molecules and non-covalent molecular assemblies. The current limitations of MS imaging techniques include sample pre-treatment prior to analysis, unwanted fragmentation of ions, and limited spatial resolution compared to optical and electron microscopy. Bringing the sensitivity and chemical specificity of MS to the nano-scale will be a major breakthrough in chemical analysis, enabling experiments that are currently unattainable. We have used PNNL's new aberration corrected transmission electron microscopes to examine a new type of silicon-carbide energy storage electrode. This study reveals how they perform better than pure silicon and how cyclic use would affect their durability. These results were published in Nano Letters in March 2012.

Advancing Proteomics to Create New Tools for High-Throughput Biological Systems Characterization. Building on a core strength in proteomics we will expand to other 'omic measurements that can more clearly reveal protein conformation, modification, activity, and interactions. Another key area is the development of complementary 'omics capabilities (metabolomics, lipidomics, glycomics, metallomics), along with the integrative data informatics and bioinformatics tools and computational methods. Focusing on high-throughput measurements on single cells for biomolecule characterization and the development of quantitatively predictive biological models, we intend to explore a variety of plant systems and their genetic variations relevant to the BER mission, as well as study new microbes and microbial communities important to hydrocarbons, hydrogen, and bioproduct production. Relevant to carbon cycling and sequestration, we are targeting terrestrial and oceanic microbial communities that play pivotal roles in carbon cycling or can serve as sentinels for environmental and ecosystem health.

Integrating Software for Image Reconstruction, Analysis, and Knowledge Extraction. New chemical imaging instrumentation must be coupled with new computational tools for real-time analysis on diverse, complex, and integrated experimental and simulation data. Effective data management will result in the creation of common ways to organize and access raw data, and extract filtered experimental observations or computational data while automatically generating the critical metadata and correlated semantics needed for quantification. New mathematical tools will map data from different experiments across spatial and temporal scales, overlay or translate images for comparative studies, and extract important features for examination. Molecular computations will model the fundamental processes that form the basis for the chemical image, providing a way to test hypothesis and scientific discovery in chemical data. Achieving experimental accuracy with computational models in near-real time will be accomplished with next generation high-performance computing resources and a broad capability-based, fast, and efficient scalable computational software that can capture dynamical processes at ultra-fast time scales. We have had several accomplishments in the development of new analytical methods for image processing, most notably in the comparison of reconstructed spatial microstructure images using different statistical descriptors. These results were published in *Computational Materials Science*.

Required Resources. This major initiative builds on programmatic leadership in BER, BES, and NIH. Some of these new capabilities will be developed at PNNL, and some will require development at accelerator-based light sources. The x-ray/vacuum ultraviolet capability will be developed at third and fourth generation light sources that possess sufficient temporal and transverse coherence (LBNL, Stanford Linear Accelerator Center, Brookhaven National Laboratory [BNL], and ANL). Development of optical, mass, electron, and scanned-probe microscope capabilities will be done in collaboration with appropriate external partners such as FEI (*e.g.*, for electron microscopy). Development of the mass microscope capability will be done in collaboration with the Netherlands Atomic and Molecular Physics Institute and the National High Magnetic Field Laboratory. The in-house development of high spatial resolution imaging tools such as the spectroscopic and electron microscopies will require dedicated (*i.e.*, non-user facility) vibrationally, electrically, and magnetically "quiet" laboratories being proposed in the new CSIL (Section 4.3). LDRD investments have been and will continue to be used to recruit additional leadership and build new capabilities in microbial communities, x-ray materials science, and multi-modal chemical imaging. Our successes over the past year include hiring Nigel Browning—an internationally recognized electron microscopist—and his group to lead our in-house imaging integration challenges, obtaining access to nine new x-ray facilities at synchrotron light sources in the United States, and several key publications including the cover article for *Analyst*.

4.2.6 Accelerating Innovation and Discovery and Transforming the Conduct of Science in the Environmental Molecular Sciences Laboratory (EMSL)

The Vision. EMSL and PNNL will develop a suite of tools to enable the dynamic understanding and control of chemical, biological, and environmental processes across space, time, matter, and energy scales. This includes constructing system level models that accurately describe and correctly predict emergent properties that occur when molecular processes drive meso-scale behaviors. More specifically these tools will be adapted to characterization of microbial and plant/microbial systems leading to manipulation of these communities to meet challenges in biofuels, energy materials, and carbon management. These tools will also be used to detect, characterize, and manipulate biological processes for threat detection and bio-stimulation for desired cellular-driven synthesis.

A necessary step in achieving the vision requires leveraging the EMSL user system to assemble cross-disciplinary teams to address these challenging scientific problems. This approach requires new ways to build teams, new incentives to promote team based recognition, and new ways to gather, analyze, store, process, and disseminate data and an innovative and interactive user facility management system that enables team cooperation and innovation.

Outstanding Scientific Challenges. The multidisciplinary EMSL Science Themes (Biological Interactions and Dynamics; Geochemistry, Biogeochemistry and Subsurface Science; and Science of Interfacial Phenomena) provide strategic direction for critical investments in the development of new technologies for innovative research as well as a focus and prioritization for user access. Although these themes and the user projects continue to guide important scientific progress, we need to build computational tools that characterize systems across scales.

The challenge before us is to build tools that provide *in-situ* multimodal characterization at the "right" scale (from nanometers to microns) of dynamic processes, and then create validated models that can accurately predict behaviors and properties at the meso (between) scale. These models must also take into account environmental responses that describe the relationship between genotype and phenotype, for example. Critical scientific challenges exist in three major areas:

Transformational Tools to Advance Scientific Frontiers. Increased data quality and relevance requires improving computational modeling, instrument resolution in all dimensions (space, energy, mass, detection limits, and time) including enabling measurements in working environments (*in situ* and in operando). Development of new predictive models along with the collection of data with higher spatial,

energy, mass, and time resolution will lead to new scientific discoveries and insights. *In situ* and operando measurements increase data relevance and are a focus of EMSL capability development (*e.g.*, EMSL's newly commissioned chemical TEM). Faster data collection and analysis will be enabled by a close coupling of theory and simulation to experiment. Making highly sophisticated advanced tools available to multi-disciplinary research teams requires the availability of experts as well as the facilities for capability development and maintenance (both computational and experimental). Some instruments already provide web-based instrument control, and we are working to increase this access while developing innovative virtual interactive user facility systems.

New Systems Understanding of Complex Interactions. The explosion in data and the computational power available to manipulate and manage it have changed the nature of science. Assembling these data in comprehensible form that is amenable to extraction of correlations and data relationships (informatics) is important as well as the ability to construct validated models to allow predictions in so called "simple" (*e.g.*, homogeneous single cell communities) and complex (*e.g.*, heterogeneous communities of microbes) systems. A robust systems level understanding of such communities requires us to predict and eventually manipulate emergent properties that arise from the complex interactions of environmental factors and the genomics of the community. For a distributed team approach to succeed, we will need to develop real-time collaborative and analysis tools that integrate distributed computational resources (from clusters to high-performance architectures) and allow asynchronous visualization including computational steering. Protecting the integrity and security of the data requires validation of distributed algorithms, balancing data integrity and security, and preserving intermediate results to maintain data provenance.

Assembling and Enabling Teams of Teams. Teams of teams will be assembled around important scientific or technological challenges. Assembling the appropriate dynamic team with the energy, enthusiasm and skills to address important problems presents many challenges, and the wide variety of freely available iPad and iPhone applications demonstrates a new model for community participation. Open Source Science is a collaborative approach for advancing scientific discovery and EMSL has formed teams around user campaigns. The development of MyEMSL furthers this end with the vision to provide the software infrastructure for the natural self-assembly of multidisciplinary teams worldwide.

Technical Approach. Building on EMSL's strengths, there are three targeted approaches:

Transformational Tools to Advance Scientific Frontiers. Significant progress has been made over the past year with more than 30 new research instruments, including specially designed environmental probes to extend instrument operations *in situ* and *in operando*. New capabilities in imaging, metabolomics, metallomics, interfacial characterization, and isotopic analysis have also been added. As an example, we have demonstrated the ability to resolve chemical shift and detailed surface interactions using high resolution SFG-VS accurate polarization/configuration dependent measurement and line shape analysis resulting in structural and dynamic information at the liquid/gas interfaces. Also, a new imaging platform (SIMS-FTICR) designed and built at EMSL has demonstrated micron spatial resolution with sufficient mass accuracy to unambiguously identify molecular species such as cholesterol in tissue samples.

Three instruments are in design: 1) high resolution and mass accuracy FTICR MS; 2) a dynamic TEM with significant time (μs) and spatial (nm) resolution; and 3) an advanced Molecular Beam Epitaxy materials deposition system. Five instruments are being specified that will significantly expand EMSL capabilities: 1) a peta-scale high performance computing architecture, 2) higher spatial- and time-resolution TEM; 3) combined magnetic resonance capabilities (electron paramagnetic, nuclear magnetic, dynamic nuclear polarization spectroscopy) expanding the range of elements and oxidation states that can be examined with one instrument; 4) integrated 'omics capabilities, including expansion of top-down proteomics capabilities, protein localization/imaging capabilities, and the sensitivity improvements required to allow single cell measurements; and 5) a compact light source for high intensity photon probing of materials and biological systems.

New Platforms for Virtual Collaborations and Data Management. MyEMSL will provide the foundational infrastructure for new platforms and protocols for data collection, processing, and sharing. The MyEMSL open-source infrastructure provides easily configurable interfaces for capturing and managing data, and is important for engaging the expertise and experience of the wider community. Currently, the MyEMSL team has activities with oreChem, CSIRO and Kitware Inc. using their open source software tools for data integration associated semantic and eventual ontological representation. Visualization is a focus for the coming year, leveraging partnerships with Scientific Discovery through Advanced Computing centers and the University of Utah.

Systems Understanding of Complex Interactions. For all three EMSL Science Themes, a systems approach will be used to bridge scales to model and understand emergent properties. For example, EMSL's new microfluidic fabrication and experimental capability is being used to generate experimental datasets for calibrating and validating pore scale numerical modeling codes and accelerate advancements in numerical modeling methodology. This is highly relevant to geochemistry but also serves as a gateway to eventual understanding of the Earth carbon cycle and stresses that will affect it. Additional specific goals are to create tools for *in situ* soil carbon and geochemistry analysis, create a library for soil organic matter, create the ability to image the root/soil/biogeochemistry interface, and model processes that effect regional systems.

In Biological Interactions and Dynamics, the goal is to develop a systems level understanding of biological systems with the potential to produce sustainable, economically viable bio-fuels. This will require a thorough understanding of cellular processes and networks, as well as signaling pathways that are critical for communities of cells to be understood and exploited. Further, the emergent properties of cellular communities, which are critical to their function, will be revealed. Specific goals are to integrate cell sorting, 'omics, and imaging data, reduce analytical detection limits to the single cell level, create metabolite libraries of targeted systems, image key cellular entities (*e.g.*, proteins) in their native environment, and create models of cellular metabolism.

Because interfaces play an important role in both environmental processes and the development of materials for energy production and storage, the objective of the Science of Interfacial Phenomena theme is focused on development of predictive models which enable the design of interfaces which optimize the performance of advanced materials systems. Specifically we will develop *in situ* molecular measurements of interfacial processes, develop theory for complex oxide surfaces and interfaces with a particular focus on understanding and characterization of liquid/solid interfaces, as these play crucial roles in many energy related (*i.e.*, batteries) systems.

Required Resources. American Recovery and Reinvestment Act (ARRA)-funded and other approved major items of equipment capital expenditures provide the foundation for new tools, but growth in EMSL user program requires commensurate growth to EMSL's operating budget. LDRD to develop the tools for building computations tools and skill sets that translate across scales will be required. In particular 'omics capabilities (proteomics, transcriptomics, and metabolomics) that push the limits of detection to the single cell level will be required to bridge scales and allow and understanding of the genotype/phenotype relationship in target communities. Other ongoing or planned investments in chemical imaging, microbial communities, climate change, carbon sequestration, materials science, signature science, and data-intensive computing may be integrated into the vision as either capabilities or team participants to help achieve the vision of accelerated discovery and innovation.

4.2.7 Simulation and Analytics

The Vision. Develop a unique set of tools and capabilities that will enable the design and exploration of advanced computing architectures for extreme scale challenges in science and security, as well as the analysis and validation of data intensive results from computational, sensor based, experimental and observational sources.

Outstanding Scientific Challenges. As computing systems become ever more complex and extreme in size, we need a fundamental understanding of their architecture and properties to develop new means to harness their power for discovery in science and security. Further, our ability to collect and generate data outpaces our ability to analyze, validate, and transform it into knowledge and innovation. Increasing volumes, rates, and heterogeneity of data produced, collected, and analyzed requires us to move our thinking beyond just the "data" and consider the challenges associated with data distributed both geographically and in terms of ownership. Tackling these challenges requires an integrated approach, reliant on fundamental computer science and mathematics capabilities in the following four areas:

Understanding the Machine. At the core of computing is the ability to understand the capabilities and constraints of emerging computing technologies and participate in the design of next-generation systems. Over the past few years we have seen a nearly equal increase in computational capabilities and accompanying constraints in their design, operation, and utilization. Power consumption, data handling, and extreme degrees of parallelism are thereby key challenges that require our attention. In designing new computing architectures we need to carefully study the tradeoffs of different solutions in terms of efficiency of operation, programmability, and optimal utilization potential for domain grand challenges. Sophisticated tools are required to support the analysis and design of new computing technologies, as well as capabilities to engineer and test new designs. Where the solutions cannot be optimized to meet all requirements, frameworks and tools that help to overcome introduced limitations and enable in efficient machine utilization are needed.

Using the Machine. With increasing complexity of computing systems, it has become apparent that the separate design of architecture, system software, and application support no longer delivers suitably optimized solutions. Instead, the path forward requires collaborative design of architectures and software tools to optimize system capabilities in terms of application utility and performance. Building on the fundamental understanding of the hardware design properties, we must develop new methodologies to control system power consumption, enable resilience of system software and user applications in more volatile computational environments, and address the handling of extreme-scale data in memory and I/O limited computer systems. To utilize these new capabilities, new programming models will be required.

Exploiting Data. With evolving technologies, we have seen significant increases in both data volumes and heterogeneity, with data from computational, sensor, observational, and experimental sources. While this data holds great promise, it is our ability to understand the data (numbers, words, or features) and convert that understanding into knowledge that truly enables progress. Discovery of implied or emerging relationships among the data permits formulation of new theories and anticipatory actions. The extreme scale and heterogeneity of the data renders many existing analysis approaches obsolete and requires us to look for novel, scalable approaches that support both data analysis and interpretation. In both science and security, the heterogeneity of the data to be analyzed and the need to identify and exploit the dependencies across data sources is a critical challenge, as is the ability to avoid the transfer of large data sets for analysis only. With large, complex data sets, the results of its analysis are often also large and complex. Consequently, it is essential that we generate methodologies and tools that allow us to effectively discover relevant details in the results of any analysis. Finally, we need to enable the capture of any new knowledge and its effective dissemination to all interested and authorized parties.

Assessing the Results. With the increasing scrutiny of scientific results new ways to assess and validate results against a background of increasing volumes of new scientific findings, from ever more complex and specialized computational and measurement techniques are needed. Transparency of processes and methods employed, reproducibility of results, and a clear assessment of the validity and uncertainty of these results are critical to the perceived veracity of scientific outcomes. Of equal importance is the ability to represent the results of such validations to both humans and machines, in forms that enable analysis and assessment across many results. We foresee specific challenges at the extreme scale, where currently available methods are no longer effective.

Technical Approach. PNNL has an extensive program of internal S&T investments and external funding for computer science research at the extreme scale. With these and a number of strategic hires, PNNL has been able to establish clear leadership in performance modeling, one-sided programming models, data intensive computing and visual analytics, and with leadership emerging in graph analytics, scientific knowledge management, and data provenance. In addressing the scientific challenges articulated above, we continue to develop and apply skills and expertise in the areas identified below.

Power, Performance, and Reliability Modeling. PNNL has extended its capabilities in modeling the performance of full applications and systems at extreme-scales with an eye toward future exascale systems. Research in model-driven optimizations has impacted system software configurations (*e.g.*, optimizing OS-jitter, network routing for InfiniBand) and application in climate, hydrodynamics, radiation transport, combustion, and particle physics domains. Extensions to this modeling capability will include both power and reliability, taking into account the power usage of various computational architecture subsystems in each phase of an application and enabling the exploration of the impact of reliability approaches on both machine performance and power usage. This open-source modeling approach supports co-design activities throughout the life-cycle of both applications and systems.

*Hybrid Architecture*s. The size of data volumes and complexity of analysis require selecting computational architectures uniquely tuned to parameters of the domain problem. Through internal investments and research programs like the Center for Advanced Supercomputing Software (CASS), PNNL is developing experience with hybrid systems that comprise heterogeneous hardware components ideally suited to accelerate components of complex analytic processes. Recent activities have explored a variety of hardware and software solutions for collecting, managing, and analyzing large volumes of cyber traffic data and social media driving both hardware and software development activities. Software infrastructure is being developed to plumb hardware and software components and seamlessly transfer data and computational requests. Going forward, power/performance/reliability modeling will be extended from the design of traditional supercomputers to embrace optimal design of hybrid computing systems to address specific domain challenges. Understanding, modeling, and designing systems characteristics will lead to more robust systems tailored to characteristics of specific domain challenges.

Programming Models. PNNL's approach to programming and execution models is derived from our long history with one-sided communication techniques which are fundamentally different from the standard two-sided (MPI) model. PNNL's unique application requirements for computational chemistry (NWChem) drove the design and implementation of one-sided communication strategies in Global Arrays (GA). While other laboratories develop domain applications (*e.g.*, physics codes) using MPI's two-sided model, this strategy was not suitable for the requirements of electronic structure calculation (sparse computational structure, load imbalance) in NWChem. GA has recently been demonstrated to run on full petascale systems (223K process run of NWChem using GA, achieved 1.39PFLOPS) and recent advances have extended GA to enable task-based execution on both homogeneous and heterogeneous computing systems while providing automatic load-balancing. We are designing new automatic code generation and optimization modules from domain-specific languages, enabling domain scientists in molecular and subsurface sciences to more easily develop computing applications that run at scale. In addition, general fault detection services for extreme-scale environments will enable fault-tolerant execution with minimal modifications to application source codes.

Scientific Knowledge Management. PNNL's development of powerful content management systems with innovative semantic extensions will enable the capture and management of knowledge, as well as the relationships between different entities. Scalable graph analytics will enable the evaluation and query of the knowledge graph and advanced inferencing algorithms to identify new discoveries. A collaborative toolkit built on this platform will enable a wide range of scientific and social media tools to utilize and contribute to the knowledge management system through well-defined APIs and protocols. New, highly componentized software architectures and federated middleware will be needed to facilitate the

extensibility and easy customization of the toolkit to enable cost effective creation of new platforms for different communities. A further research focus will be the investigation how such a framework can address similar challenges present in the security domain.

Complex Graph and Network Analytics. PNNL is a leader in the application of multithreaded systems to graph and network analysis problems with active research technologies for discovering hidden relationships and predicting future events. Activities under CASS are informing the development of new algorithms and system software for analysis of complex networks and semantic analysis. CASS is driving the design of new computing architectures to support a range of graph and network analysis problems. Its work in discovery of emerging relationships in heterogeneous data sets will transform the way analysts work; allowing them to predicate events before they happen rather than react to them after they happen. CASS is developing next generation semantic technologies to process temporal and spatial queries on complex data sets. User scenarios across broad domains are establishing new requirements for query languages, search engines, and data management systems.

Visualization. Leveraging unique strengths in information visualization, PNNL continues to expand its research activities in multimedia analysis and visualization of highly structured data. PNNL will expand its capabilities in extracting and linking features in heterogeneous data and developing interactive visual representations of those relationships. Emphasis on visual analysis algorithms that that can be expressed in platforms ranging from low-power, fieldable devices to high performance computing environments will provide access to analytic capabilities across domains and new user experiences for scientific discovery. Through analytics-as-a-service offerings, PNNL will deliver information analysis capabilities to users in ways that offer greater deployment efficiencies and usability. Further, by linking its HPC and information visualization capabilities, PNNL will create performance and scale benefits that have previously been the province of traditional scientific visualization, including the creation of visualization systems for exploring the results of large-scale climate simulations through exploitation of GPU-based acceleration. New research in visual aids to situational awareness in the power grid will bring synthesized views of heterogeneous information (including grid behavior, security, weather, economics, and socio-behavioral models) to operational, planning, and policymaking communities to advance the development and management of the future power grid.

Assessment and Validation at Scale. Uncertainty characterization will limit the assessment scope by determining a clear context for the assessment as well as critical factors for the validity assessment of results. Provenance at scale will provide the ability to track and analyze the history of any data, which will be enabled through more compact provenance formats; creation and analysis of large causal graphs representing different actors in the creation process and their relationships; and multi-level representation and exploration capabilities for provenance data. Uncertainty quantification for computational and observational data in complex systems will determine the uncertainty of results within a given context by developing scalable algorithms and solvers for quantifying uncertainty across multiscale, multi-physics models, observation data uncertainty and signature discovery from petascale data sets, and developing scalable solvers for uncertainty quantification on DOE leadership computing platforms. Classical validation, the comparative analysis with reference results, will be supported by adaptable data transformation infrastructures and machine learning techniques for the generation of synthetic test and evaluation data sets. Further analytical methods will be used to combine overall results of the three different methods into representations that can be easily explored by both humans and machines.

Required Resources. Computing at PNNL builds on many years of strong programmatic investment in the areas of analytics and high performance computing, where it has attained leadership positions in visual analytics, graph analytics, programming models, complemented by more recent leadership in performance and architectures. Further, PNNL has internal investments to build a leading computing and data analysis infrastructure for its staff, able to flexibly support both programmatic and internal research needs. PNNL is well positioned to make its mark in the new themes of exascale computing and data

intensive science and to realize the full potential a number of supporting investments are needed, including continued LDRD support for the extreme scale computing initiative; support for PNNL exascale development work through sizable local computing systems (target: 10% of ASCR leadership class computing facilities); and creation of critical new capabilities in analytics for distributed data to advance research capabilities and support key hires in data-intensive analytics, visualization, and software architectures. Close coordination with similar potential investments in cyber, molecular science, signature discovery, and power grid will provide demonstrable results in multiple domains of interest. Lastly, new senior hires in visualization, data intensive analytics, programming models, and uncertainty quantification will provide additional leadership and enable PNNL to grow existing programs and address computing challenges significantly and open the opportunity to lead in new major areas, such as ASCR extreme scale data sciences, BES facility software infrastructure developments, and BER Climate Knowledgebase.

4.3 Setting the Stage for Success: People and Places

The Laboratory is working aggressively to advance these seven major initiatives, each of which leverages programmatic work and Laboratory investments in foundational research and advanced technology development. In particular, internal investments are being made to attract additional scientific leaders in imaging, materials, and computing. Our comprehensive approach to attract, develop, and retain scientific staff is described in Section 7, while several of our exemplary staff and their accomplishments are highlighted on page vi. More generally, the Laboratory's LDRD portfolio is reviewed regularly as a part of the strategic planning process, and adjustments are made to accelerate progress on these initiatives in order to maintain the core capabilities critical to future mission readiness.

New facilities will be needed to realize the Laboratory's scientific vision. Our facility strategy continues to mature and is fully discussed in Section 6. The new facilities essential to the mission readiness of our core capabilities and the success of the major initiatives are:

- *Chemical Sciences and Imaging Laboratory*. This facility will provide unique capabilities to transform the way chemicals and materials are synthesized and studied, including for the development of energy storage materials, alternative fuels, and systems for carbon capture and sequestration. Utilizing specialized quiet space for new multi-modal imaging tools—space that does not currently exist at PNNL—the CSIL will enable the synthesis of new nano-structured, multi-functional catalysts; the observation and imaging of catalytic processes with atomic resolution, *in operando*; and the coupling of theory and modeling activities to predict catalytic behavior over multiple orders of magnitude time-scales and distances. The current schedule does not support the mission readiness needs of our core technical capabilities or our scientific vision.
- *Power Engineering Research Laboratory*. The Power Engineering Research Laboratory (formerly the National EIOC) will be DOE's national grid modeling, monitoring, and analysis facility focused on developing the knowledge that enables the next century of progress for U.S. electric infrastructure. Through sensor data collection and analysis, this Laboratory will enable real-time visualization of the national electric grid at the interconnection scale. This Laboratory, which we expect to be built in partnership with the State of Washington, UW, and WSU will be a test bed for evaluating new grid technologies and operation opportunities and will showcase the results of the grid and data-intensive computing initiatives.
- *300 Area Transition – Phase II*. Our focus in FY 2013 remains on the planning required for Phase II of our transition out of the Hanford Site 300 Area. Currently, there is approximately 300,000 gsf of highly-specialized radiological and nuclear laboratory space in the Hanford Site 300 Area that we are expected to vacate by 2026. Given the magnitude of the challenge to provide modern, replacement laboratories to keep our core capabilities in applied nuclear science and technology, applied materials science and engineering, and subsurface science fully mission ready, planning for a Critical Decision (CD)-0 in

FY 2014 continues. Given the highly specialized, high hazard class nature of these laboratories, we expect the replacement facilities to be funded with federal funds and sited on federal land.

- *The Center at PNNL*. The Center at PNNL is a staff and visitor collaboration facility that will provide a collaborative working environment and improve PNNL's ability to meet the primary mission of scientific discovery. Over the last decade, PNNL has added nearly 1000 additional permanent staff, nearly doubled its overall business volume, and increased the core campus staff density by approximately 30 percent. The growth in the number of staff on campus and increase in staffing density has occurred without concurrently accommodating meeting and collaboration spaces that are typical for organizations of the size and prestige of PNNL. The Center at PNNL will provide an on-campus meeting and collaboration experience consistent with the Laboratory's cutting-edge discoveries and exceptional research programs. The Center will supply new space to increase S&T staff collaboration and productivity, provide opportunities to host significant scientific and technical conferences, and offer more flexible and functional meeting spaces.

5.0 Work for Others

The Work for Others (WFO) program creates opportunities to leverage non-DOE federal and non-federal resources to accelerate scientific discovery and deploy solutions that benefit both DOE and the sponsoring entity. WFO projects are a strategic component of the Laboratory's research portfolio that together, represent a larger, coordinated set of activities that address a national need across multiple agencies. In many instances, the WFO project is as essential as the DOE-funded activities. Leveraging DOE and WFO activities enables PNNL to deliver national solutions cost-effectively, and provides opportunities to advance our scientific vision, fuels progress on major initiatives, and enhances our core capabilities. A summary description of PNNL's WFO activities is included in Appendix 1.

5.1 Baseline WFO Program

PNNL has furthered DOE's energy and science mission through participation in extramural research funded by the Defense Advanced Research Projects Agency (DARPA), NASA, and the U.S. Army aimed at developing the hydrogen economy and energy storage options. Through DARPA and Army-supported research and development efforts focused on the development of microchannel reactors for man-portable and remote/wireless fuel cell applications, PNNL researchers have advanced DOE/EERE programs by developing new fuel reforming catalysts and fuel processors for onboard and transportation applications, as well as DOE-SC programs that provided a fundamental understanding of nanostructured catalysts for hydrogen production from renewable resources. Under DARPA supported research on the development of novel membranes for lithium ion batteries, PNNL has advanced DOE-OE programs in the development of next-generation lithium ion-based batteries.

PNNL researchers work with DoD and the nonproliferation community to develop and deploy world-class ultra-trace analytical radiation detection and MS expertise linked to DOE's national security mission. This work has been ongoing for more than 40 years and is integral to PNNL's Signature Discovery and Exploitation for Threat Detection and Reduction major initiative. DoD has provided funding for instrumentation and laboratory modifications that have advanced PNNL's core capabilities in nuclear science and technology and systems engineering and integration.

PNNL research in data-intensive computing supports DOE's missions in national security and scientific discovery and innovation. The Center for Adaptive Supercomputing Software conducts research on massive multithreaded architectures, semantic databases, and graph algorithms for data-intensive applications. In 2011, the Center organized international workshops in irregular applications, graph libraries, and semantic database search patterns. It maintains extensive partnerships with other national laboratories, industry, and academia, and has enhanced PNNL's capabilities in a variety of data-intensive sciences. ASCR and other DOE offices, such as DOE-FE and DOE-OE, leverage this work to accelerate programs in data-intensive sciences, cyber-analytics, carbon capture simulations, and power grid modeling.

PNNL has furthered DOE's mission of scientific discovery and innovation through participation in the NIH extramural research program. Using novel MS-based methods, PNNL researchers are developing models of metabolism for bacterial pathogens, improving genome annotations based on proteomics results, and elucidating host-pathogen interactions. This work has advanced DOE-BER programs by developing modeling and prediction capabilities for DOE relevant microorganisms, microbial communities, and novel genome annotations. PNNL core capabilities support BER genomic science, low dose radiation, subsurface biogeochemical processes and terrestrial carbon sequestration research programs.

The current portfolio of WFO clients and funding levels is shown in Table 1. Over the past 5 years (2007–2011), WFO programs (excluding DHS) have averaged 15% of the work performed and are expected to be 18% in FY 2013.

The diversification of PNNL's research portfolio enables the Laboratory to remain flexible and maintain mission ready capabilities. WFO-funded programs also help defray the fixed costs associated with the management and operation of the Laboratory, contributing approximately $70M to institutional and organizational overhead pools in FY 2011. As a result of this cost sharing, the Laboratory is able to deliver more research and development per dollar invested.

Table 1. Work for Others Funding Budget Authorization in ($M)[1]

Sponsors	FY 2011 Actual[2]	FY 2012 Estimated	FY 2013 Request
DoD	$60.8	$52.0	$53.4
NRC	$19.6	$19.1	$22.5
DHHS/NIH	$20.8	$21.4	$21.4
All Other Federal Work	$77.1	$64.2	$66.4
Non-Federal Work[3]	$13.2	$26.8	$33.0
Total WFO[4]	**$191.6**	**$183.4**	**$196.6**
Lab Operating[5]	$875.7	$991.7	$1,057.0
WFO as % of Lab Operating	**22%**	**18%**	**18%**
DHS	$59.7	$58.9	$60.3
WFO + DHS as % of Lab Operating	**29%**	**24%**	**23%**

[1] Numbers are for planning purposes only.
[2] Includes funding received as part of the ARRA.
[3] Includes projected impact of some Use Permit work transitioning to Non-Federal WFO. We are working to transition the Use Permit work to Agreements for Commercializing Technology ([ACT] $14M in FY12; $35M in FY13), as appropriate. These numbers will be provided in the future plan.
[4] Does not include DHS funding when computing the Total WFO funding level.
[5] Refers to funding programs and others sent to the laboratory to perform R&D, etc., including capital equipment and General Plant Project (GPP), but excluding construction.

5.2 WFO Strategy for the Future

WFO projects are thoroughly reviewed for strategic alignment through PNNL's institutional strategic planning and risk acceptance processes. Project teams identify the critical science and technology challenges and consider alignment with institutional strategy and customer expectations and relationships. The teams also assess potential risks, including risk to reputation and the potential to strain critical scientific and technical capabilities or critical infrastructure before accepting WFO projects.

The Laboratory's WFO programs do not put undue strain on critical scientific and technical capabilities. There are none so large that the reduction/termination of the program would require significant staff terminations; they do not require the use of significant discretionary resources to support specialty infrastructure not already and primarily driven by DOE or DHS missions, nor are there any that involve a level of subcontracting not appropriately balanced by the research content of benefit to DOE.

The optimal WFO portfolio is one that delivers national impact while complementing DOE's multiple missions and nurturing the Laboratory's core capabilities. Our strategy is to leverage funding—wherever available—to accelerate scientific discovery and innovation.

PNNL will take a leadership role in DOE's three-year pilot ACT to facilitate interaction between the national laboratories and commercial entities for the purpose of increasing the pace and impact of technology transfer. A good example is in the development and integration of large, grid-scale energy storage devices. PNNL has a strong IP portfolio in several promising technologies, including vanadium redox flow batteries. These batteries can greatly enhance grid functionality and reliability and support the integration of renewable generation resources. Private industry recognizes PNNL's strength, and we anticipate private companies will be making arrangements to work with PNNL and invest in developing commercially viable batteries.

6.0 Infrastructure/Mission Readiness

6.1 Overview of Site Facilities and Infrastructure

PNNL is located in Richland, WA with several offsite locations. The main PNNL campus located at the north end of Richland consists of land owned by DOE, Battelle, and third parties. Utilities infrastructure is owned, operated, and maintained by DOE and the City of Richland. They remain in fair to good condition with several new fiber cables installed in FY 2011 to mitigate end-of-life failure. The facility profile comprises 96 buildings, including:

- 19 buildings owned by DOE (830,803 sq ft; average age of 20 years)
- 41 buildings owned by Battelle (390,992 sq ft; average age of 34 years)
- 36 buildings from third-party leases and agreements (1,111,048 sq ft; average age of 24 years).

All PNNL Hanford 300 Area buildings were transferred to the Hanford Site cleanup contractor during the second quarter of FY 2011, with the exception of 325 (RPL), 331, 318 (RCL), and 350 buildings, which will be retained for PNNL use until approximately 2026, in accordance with the Memorandum of Agreement between SC and EM.

PNNL's real estate actions during FY 2011 and FY 2012 consist of one 48,000 gsf new lease, one 16,000 gsf new inter-laboratory agreement, and five lease renewals (over 10,000 sf each). Specific to FY 2012/2013, the BMI-owned facilities will transition to DOE leased facilities. Continuing with the campus master plan strategy, PNNL plans to consolidate research activities to the core campus, which has the potential to reduce the lease facility footprint over the five-year planning period. A summary of the near-term lease actions, the leased facility footprint and the current five-year expiration timeline can be found in Appendix 5. Site land use is described in the PNNL Campus Master Plan.[(1)] Table 2 includes the SC buildings and Hanford Site EM buildings totally occupied and maintained by PNNL. Asset Utilization Index values were calculated from Facility Information Management System data validated March 2012.

Table 2. PNNL's DOE (EM and SC) Currently Owned and Operated Facilities and Infrastructure – FY 2012 Data

			Total Bldg, Trailer, and OSF RPV ($; less 3000 Series OSFs)				$409,483,904
			Total OSF 3000 Series RPV ($)				$0.00
FY 2012 Site Infrastructure Data Snapshot			Total RPV ($)				$409,483,904
Secretarial Office	SC		Total Deferred Maintenance ($)				$2,120,624
Field Office	Oak Ridge Office		Total Owned Acreage				346
Site	PNNL		Total Leased Acreage				0
Year	2011		Site-Wide ACI (B, S, T)				0.995
			# Bldg Assets	**# Trailer Assets**	**# OSF Assets**	**GSF (Bldg)**	**GSF (Trailer)**
Asset Condition Index (B, S, T)[1]	Mission Critical	0.996	10	0	1	766,586	0
	Mission Dependent	0.975	2	3	8	42,140	7,253
	Not Mission Dependent	1.000	4	0	1	4,694	0
Asset Utilization Index (B, T)[2,3]	Office	91.69	1	3		700	7,253
	Warehouse	100	3	0		21,264	0
	Laboratory	95.12	9	0		765,886	0
	Hospital	0	0	0		0	0
	Housing	0	0	0		0	0

B=building, OSF=other structures and facilities, RPV=replacement plant value, S=structure, T=trailer
[1] Criteria includes DOE-owned buildings, trailers, and OSFs (excludes series 3000 OSFs)
[2] Criteria includes DOE-owned buildings and trailers
[3] Only includes assets with usage codes that fall into these FRPC categories; other usage types are not included
[4] Does not include leased facilities
Note: FIMS data in the table (as of 3/1/12) differs from the 2011 year-end FIMS report, which contained a $200M single data entry error.

[(1)] http://facilities.pnl.gov/resources/fsp/PNNLCampusMasterPlan_0109.pdf

6.2 Facilities and Infrastructure to Support Laboratory Missions

Consistent with the PNNL Campus Master Plan, current and planned investments have sought to establish a modern, sustainable, collaborative and flexible campus in support of the core capabilities. During FY 2010 and FY 2011, PNNL successfully addressed the first of the three main drivers of our facility and infrastructure strategy, with the implementation of the Phase I transition out of the Hanford Site 300 Area. The transition provided significant improvements to portions of the biological systems, advanced nuclear science and technology, applied material science and engineering and advanced computer science, visualization and data core capabilities.

The second major driver of our strategy is the continuing need to modernize the remaining facilities and infrastructure on PNNL's Campus. Campus modernization supports the expanding impact of the EMSL user program by increasing access to EMSL capabilities, and supports the increasing demand for our applied materials science and engineering, chemical engineering, and chemical and molecular sciences core capabilities that are central to our world-class science in catalysis.

Significant progress was made on this task in FY 2011 and continues in FY 2012 with the implementation of a detailed five-year plan for campus modernization. This plan was driven by an analysis of the mission readiness of our core capabilities, particularly in facilities and infrastructure. The results of this analysis are shown in Appendix 3, which details the facilities and infrastructure mission readiness and planned investments for all of our core capabilities, and Appendix 4, which shows the mission readiness of our support facilities and infrastructure. A summary of our key strategic investments in relation to the core capabilities can be found in Table 3 below.

Table 3. Current and Planned PNNL General and Scientific Infrastructure Investments

Project Title	Core Capability	Facility	Year Planned	Summary Scope
CRL-II	• Applied Nuclear Science & Technology • Applied Materials Science & Engineering • Chemical Engineering • Environmental Subsurface Science • Chemical & Molecular Science • Biological Systems Science	New facility Line Item funded	10+ years	Replace radiological and nuclear facilities in the 300 Area in order to vacate by 2026
CSIL	• Chemical & Molecular Science • Biological Systems Science • Environmental Subsurface Science • Applied Materials Science & Engineering	New facilities Line Item funded	Within 5 years	Provide centralized and modern laboratory spaces to support the following research activities: • Imaging and analytical • Wet chemistry • Large scientific instruments
Power Engineering Research Laboratory	Systems Engineering and Integration	New facility Institutional General Plant Project (IGPP) funded	Within 5 years	Support real-time monitoring of the national electric grid
The Center	NA	New facility IGPP funded	Within 5 years	Provide a conference room, welcome center, and cafeteria amenities
Campus computing consolidation projects	• Advanced Computer Science, Visualization and Data • Large-Scale User Facilities/Advanced Instrumentation	CSF, EMSL and new facility IGPP funded	Within 5 years	Consolidate unclassified programmatic computing, centralize classified computing and build a new data center to support the campus needs
R&D Lab Optimization	• Biological Systems Science • Chemistry & Molecular Science • Environmental Subsurface Science • Applied Materials Science & Engineering • Applied Nuclear Science & Technology • Systems Engineering & Integration	Multiple projects spanning 325 (RPL), 331, LSL-II, RTL, PDLW, 3420, 3410 IGPP funded	Within 5 years	Various upgrades to laboratory configurations

While the PNNL facility footprint on the South Core Campus is well maintained and provides safe, secure, and reliable operations to research programs, the space is fully subscribed and facing increasing demands from programs that are strategically important to DOE and the nation. Moreover, this space has not kept pace with the changing face of science in the 21st century. In all buildings, collaboration space has fallen well below industry design standards as conference rooms and other office support space has been used to house staff. In addition, with the exception of EMSL and parts of the newly constructed PSF, PNNL's non-radiological laboratory space was constructed during the mid-1960s and early 1970s and since that time research technology and operations have changed significantly. Original laboratory building designs now encumber research productivity and collaboration.

In some cases, functionality now common to scientific laboratory facilities, such as highly specialized vibrationally, electrically, and magnetically "quiet" laboratories for multi-modal imaging tools, and modern synthetic chemistry laboratories, exist only as part of the EMSL user facility, with priority given to user programs. This affects our chemical and molecular sciences, chemical engineering and subsurface science core capabilities, as well as the *In Situ* Chemical Imaging and Analysis and Controlling Interactions Across Scales to Enable Scalable Synthesis major initiatives. The need for this highly specialized space, along with fume hood intensive synthesis laboratories, is driving our SLI request for the CSIL.

The third major driver of our facility strategy is the need to continue planning for Phase II of the 300 Area transition. With the completion of the CRL and 300 Area life extension projects, PNNL has 300,000 gsf of highly specialized radiological and nuclear laboratory space remaining in the Hanford Site 300 Area that we are expected to vacate no later than 2026. Due to the magnitude of the challenge to provide modern, replacement laboratories to keep our core capabilities in applied nuclear science and technology, chemical engineering, chemical and molecular science, applied science and engineering, biological systems, and environmental subsurface science fully mission ready, CD-0 planning has begun for Phase II of this transition. Given the highly specialized, high-hazard class nature of these laboratories, we expect these replacement facilities to be federally funded and sited on federal lands.

In the following section, we describe in detail some of the actions already taken to address our facility strategy drivers and outline what we need from DOE in order to keep our core capabilities mission ready, achieve our scientific vision and solve problems in energy, the environment, and national and homeland security critical to DOE and the nation. PNNL's assessment process, which includes an evaluation of all facility and infrastructure investments against impact to mission readiness and strategic alignment to core capabilities, was reviewed in FY 2012. Our process continues to mature with elements considered best practices and may be applicable to the entire family of national laboratories.

6.3 Strategic Site Investments

PNNL is committed to keeping its core capabilities mission ready. We have been successful, in part, at responding to the increasing demand for these capabilities by programs of strategic importance to DOE and the nation by aggressively and comprehensively managing our costs (see Section 8.0). In turn, those savings have been channeled into strategic investments, which have nearly tripled the capital investments (through IGPP) since FY 2008, to optimize current facilities and provide new, modern laboratory facilities to enable scientific excellence in the 21st century.

6.3.1 Campus Modernization

Three efforts are essential to PNNL's campus modernization efforts: evaluation and optimization of existing facilities; acquisition of space; and construction of new specialized isolation and chemical synthesis space. The first is critically examining our existing facilities and making investments necessary to increase the efficient, effective use of the laboratory space in high demand (particularly chemistry, radiochemistry, and radiological) in PSL, RCL, RPL and RTL. These optimization projects advance

mission readiness for applied material science and engineering, subsurface science, and applied nuclear science and technology core capabilities and benefit programs for SC, EERE, NE, EM, NRC, FE, USACE, NNSA, DHS, and the Intelligence Community. Additionally, the RCL and RPL projects will address a portion of the Signature Discovery and Exploitation for Threat Detection and Reduction major initiative resource requirements.

Using our existing space more efficiently, however, addresses only a small portion of the scientific demand for specialized laboratory space such as imaging and wet-chemistry space. A review of ongoing projects did not identify any space that could be reprogrammed to provide this specialized laboratory space without adversely affecting programs of strategic importance to DOE or the nation. Consequently, the second major effort is focused on the acquisition of space. Planned acquisitions will support the expanding impact of the EMSL User Program by providing sufficient swing space to upgrade and modernize our existing laboratory facilities, and enable real-time monitoring and operation of the U.S. electric grid. The facility acquisition will provide a national modeling, monitoring, and analysis facility to support a broader spectrum of research in order to plan and operate the U.S. electricity infrastructure in ways not possible today. The facility need aligns to the Efficient and Secure Electricity Management from Generation to End Use major initiative (see Section 4.3). These acquisitions will enable the chemistry-based and systems engineering and integration core capabilities. Battelle and DOE have incorporated the Life Sciences Laboratory II (LSL-II), a Battelle-owned facility on the Campus as a part of the pending Battelle-owned facilities lease. The addition of LSL-II is an initial step in addressing needed swing space to upgrade and modernize our existing facilities and reduce our off-Campus leased facilities footprint. We are evaluating additional options to upgrade and modernize laboratories that support our chemistry-based core capabilities and expand the impact of the EMSL User Program. Additionally, for the purpose of accommodating the growing need for conference room space, an on-site cafeteria, and welcoming center, a new facility acquisition has been included in the facility strategy. The new acquisitions anticipate funding from IGPP dollars.

6.3.2 Chemical Sciences and Imaging Laboratory

The third and most important major effort is construction of the CSIL facility to provide specialized isolation and chemical synthesis space critical to achieving PNNL's scientific vision, which requires interdisciplinary and collaborative teams of world-class scientists and engineers working in modern state-of-the-art research facilities specifically designed for science in the 21st century. The CSIL will provide mission-critical space, including:

- Dedicated, modern, electromagnetic force, acoustic-, and vibration-isolated (*i.e.*, quiet space) special purpose laboratories for state-of-the-art imaging and analytical capabilities. This space would provide isolation from noise that can negatively impact the performance of new-generation imaging instruments (*e.g.*, aberration-corrected TEMs; *in situ* scanning-probe microscopes; other atom or nanometer-scaled probes for tomographic or structural determinations).
- Centralized modern fume-hood-intensive, wet chemistry space for fine molecular chemical synthesis and nano-phase materials synthesis.
- Adaptable, high-ceiling, high-clearance space for large scientific instruments (nuclear magnetic resonance, chemical physics) and bench-scale chemical reactors for chemical engineering.

The new construction enables PNNL to accelerate research in catalysis science and emissions engineering by combining research and facility capabilities that focus on making, measuring, observing, and modeling new materials for clean energy production. Many core capabilities will benefit, as will several major initiatives, including Controlling Interactions Across Scales to Enable Scalable Synthesis, *In Situ* Chemical Imaging and Analysis, and Coupling Earth and Energy Systems for Sustainability.

The challenge is that the CSIL, originally scheduled for construction starting in 2013 as an SLI line item, has now slipped to 2019. This schedule does not support the mission readiness needs of our core

capabilities or the achievement of our scientific vision, and we are working with DOE in accordance with Order 413.3b to address this. The project has met the requirements of CD-0 and received approval of the Mission Need Statement (MNS) by the Energy Secretary Acquisition Advisory Board on December 1, 2011. We are proceeding with the alternatives analysis to develop a recommended alternative for resolving the gap defined in the MNS.

In summary, as a result of our aggressive prioritization of work and optimization of our existing space—enabled by our disciplined cost control efforts—we are fully utilizing our facility functional capabilities. However, the construction of CSIL and access to the LSL-II facility are essential to the continued modernization of the PNNL campus. Without these facilities the gap between facility functionality and the demands of our modern research enterprise will continue to grow.

6.3.3 300 Area Transition – Phase II

In FY 2011, Phase I of PNNL's transition out of the Hanford Site's 300 Area was accomplished with CRL and 300 Area facility life extension project completion. This leaves 300,000 gsf of highly specialized radiological and nuclear laboratory space in the 300 Area that we are expected to vacate no later than 2026. With the magnitude of the challenge to provide modern replacement laboratories to keep our core capabilities in applied nuclear science and technology, chemical engineering, chemical and molecular science, biological systems science, and environmental subsurface science fully mission ready, CD-0 planning has begun for Phase II of this transition. Given the highly specialized, high hazard class nature of these laboratories, we expect these replacement facilities to be federally funded and sited on federal lands.

6.3.4 Facility Computing Strategy Projects

In FY 2012, PNNL commissioned a team to establish a strategy for developing, maintaining and investing in computing facilities. The facility strategy consists of consolidating computing into a few energy-efficient locations, prioritizing the on-campus datacenter for distinctive capabilities and providing flexible and expandable infrastructure to meet the growing needs of the advanced computer science, visualization and data core capability. In the near-term, facility investments would focus on consolidating unclassified R&D programmatic computing into one facility and building out a portion of CSF to support SCIF High Performance computing. Long-term investments consist of optimizing existing space in EMSL, migrating PNNL core computing to one location and building a new datacenter facility to support the campus needs. Funding will be provided by IGPP overhead dollars. These investments will support the PIC program by providing the research community access to a centralized computing service.

6.3.5 Facility Maintenance

Key elements of the maintenance investment plan over the next five years includes upgrading failing heating systems, fume hood replacements and end of life roofs for facilities in the core campus. The strategy to reduce deferred maintenance is to provide continued funding for planned maintenance, fund F&I initiatives to repurpose the core campus and complete the major investments described above.

6.4 Trends and Metrics

PNNL's Mission Readiness Assessment Process is fully implemented. Within that process, the PNNL facility and infrastructure maintenance program has been cited as a strength in peer review and DOE maintenance program assessments. Investment planning for this program combines component-based maintenance forecasting with real-time condition inspection and performance data to maintain facilities and infrastructure across their life cycle, minimizing deferred maintenance and operating with a high degree of reliability. The approach is consistent across the SC, EM, and Battelle-owned buildings PNNL occupies.

Over the past few years, ARRA funding has focused on energy efficient improvements to the PNNL campus. In FY 2011, the following projects were completed: installation of photovoltaic electric vehicle charging stations at EMSL, irrigation system improvements, and zero-scape installation at the 331 Building.

The transition from 300 Area facilities to new facilities (3410, 3420, 3425, 3430 and 3440) plus building life extension investments in 318, 325, and 331 coupled with planned maintenance and renewal will continue to keep deferred maintenance manageable. From a maintenance perspective, the facility and infrastructure condition is fully able to support PNNL's core capabilities. The asset condition index for PNNL DOE owned and operated retained facilities and infrastructure remains at 1.0 (excellent) through the planning period. Planned levels of investment are shown in Table 4 and Figure 2.

Table 4. PNNL's SC Owned and Operated Facilities[1] and Infrastructure Investments ($M) – Impact to Asset Condition Index (FY 2013–2022 IGPP values pending EC's FY 2013 guidance/decision)

$M	FY 2011	FY 2012	FY 2013	FY 2014	FY 2015	FY 2016	FY 2017	FY 2018	FY 2019	FY 2020	FY 2021	FY 2022
Maintenance	8.9	6.6	8.0	9.3	7.4	7.9	14.8	8.2	7.2	11.8	8.1	11.3
Deferred Maintenance Reduction	0	0	0	0	0	0	0	0	0	0	0	0
Excess Facility Deposition	0	0	0	0	0	0	0	0	0	0	0	0
IGPP[2]	13.0	9.0	13.6	13.1	9.6	12.5	21.0	18.0	12.0	12.0	12.0	12.0
GPP[3]	7.7	4.6	3.3		9.0	9.0			9.0	9.0		
Line Item[4]									10.0	33.0	50.0	0.5
Total Investment	**29.6**	**20.2**	**24.9**	**22.4**	**26.0**	**29.4**	**35.8**	**26.2**	**38.2**	**65.8**	**70.1**	**23.8**
Estimated Replacement Value	409	420	430	441	452	463	475	487	499	511	524	632
Estimated Deferred Maintenance	2	2	2	1	1	1	1	1	1	0	0	0
Asset Condition Index	0.99	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

[1] Does not include any leased facilities
[2] IGPP includes planned investments in DOE leased facilities
[3] GPP details represent EMSL programmatic investments. Planned investments consist of a central power plant in FY 2015, an office pod in FY 2016, a computer room in FY 2019 and second office pod in FY 2020.
[4] Line Item funding is reserved for CSIL pending decision; see discussion in 6.3.1.
Note: FYs represent when they expect to receive funds; actual construction/consisting may be plus or minus a year.

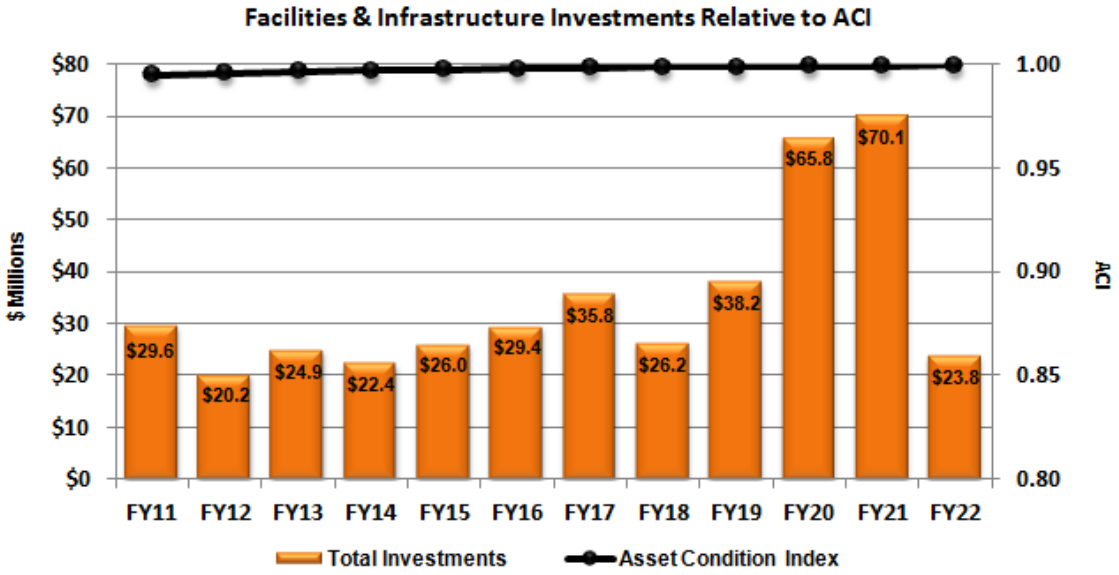


Figure 2. PNNL's Facilities and Infrastructure Investments

6.5 Sustainability

Sustainability at PNNL means thinking holistically about the impact of our operations against the "triple-bottom-line" of environmental stewardship, social responsibility, and economic prosperity. Our vision is to be recognized as a thought leader in sustainability by our customers, our employees, and the community. Our solutions – in both research and operations – will be sought out and used to make the world a more sustainable place. Every employee will be empowered to improve our sustainability performance, enabling us to achieve our aggressive goals.

Our strategy for meeting the sustainability goals are outlined in our Site Sustainability Plan. This comprehensive approach to fulfilling Executive Order 13514 will advance the DOE sustainability mission with a diverse approach and a concentrated effort towards the goals of FY 2020 and beyond. Our plan includes practical actions that can be taken to save energy and money, improve the comfort and productivity of employees, and benefit the environment. In FY 2011, PNNL reduced its combined Scope 1, 2, and 3 GHG emissions by 1.7%. Highlighted areas of achievement include energy intensity reduction, potable water use, high performance sustainable building (HPSB) areas, and renewable energy sources:

- Energy Intensity Reductions – Between FY 2003 and FY 2011, energy efficiency projects, operational improvements, and transitioning of work from aging to modern facilities have helped offset energy use increases from additional staff and equipment. At the end of FY 2011 energy intensity at PNNL is 155 kBtu per GSF, a net 21.6% toward the 30% energy intensity reduction goal.
- Potable Water Use – PNNL achieved the FY 2020 26% water intensity reduction goal during FY 2011. Implementation of water saving projects, a significant reduction of potable water used for irrigation at the 331 Building, and operational improvements from advanced meters contributed to an overall water intensity reduction of 53% compared to the FY 2007 baseline.
- High Performance Sustainable Buildings – In the area of high performance sustainable buildings, we have matched and exceeded DOE's goal for 15% of existing buildings, meeting the five Guiding Principles. Currently 25% of PNNL buildings meet the HPSB goal. In FY 2012, PNNL will certify three additional buildings and plans for two additional buildings being certified by FY 2013.
- Renewable Energy – During FY 2011, our on-site 125 kW photovoltaic (PV) array provided 136.3 MWh of electricity to our super-computing facility and adjacent car charging stations. PNNL will work with regional and federal stakeholders in FY 2012 to evaluate opportunities for a large-scale renewable power project on federal land (the Northwest Energy Initiative).

Over the last 2 years, PNNL has developed a strong framework for the review, tracking, and reporting of sustainability goals. Laboratory management also recognized that opportunities exist to institutionalize sustainability into decision-making processes and increase staff awareness on how their day-to-day work impacts the Laboratory's sustainability performance. Working groups were formed, focusing on Scope 1, 2, and 3 GHG emissions. The project goals were to improve conservation and energy efficiency in buildings/data centers (GHGs and energy) and reducing employee commuting and business travel at the Laboratory. Working group representatives included employees from a variety of stakeholder groups, including R&D, Human Resources, Information Technology, Facilities and Operations, and Business Development. The working groups analyzed the current state of how the buildings/data centers were operating and employee commuting and business travel. Results of those sessions identified opportunities to impact emissions. The recommendations from the working group are currently being evaluated by Laboratory management for implementation beginning in FY 2012, and progress is indicated in Table 5.

Table 5. Progress Toward Attaining SC Sustainability Goals

SSPP Goal #	DOE/SC Goal	Performance Status	Planned Actions and Contribution	Non-attainment Risk (H, M, L)
1.1	28% Scope 1 & 2 GHG reduction by FY 2020 from a FY 2008 baseline	FY 2008 Baseline: 36,007 $MTCO_2e$ FY 2011 Actual: 42,719 $MTCO_2e$ (11,381 $MTCO_2e$ adjusted for RECs) FY 2020 Goal: 25,925 $MTCO_2e$	Our Renewable Energy Certificates (REC) purchase strategy contributes toward the GHG reduction goal, but as a near-term strategy. This approach offers time to identify resources to implement a comprehensive plan for energy conservation, including core business hours and aggressive real-time commissioning.	M
1.2	30% energy intensity reduction by FY 2015 (FY 2003 baseline)	FY 2003 Baseline: 197,970 Btu/gsf FY 2011 Actual: 155,400 Btu/gsf FY 2015 Goal: 138,579 Btu/gsf	Continue implementing consolidated energy data report projects and operational improvements to obtain the 30% energy savings by 2015.	L
1.5	7.5% of annual electricity consumption from renewable sources by FY 2013 and on (5% FYs 2010–2012)	On-site generation and REC purchases accounted for 61.8% of PNNL annual electrical consumption in FY 2011	PNNL plans to continue operating our 125KW on-site PV array and purchasing RECs to meet this goal.	L
1.7	2% annual reduction in fleet petroleum consumption by FY 2020 (FY 2005 baseline)	FY 2005 baseline was 37,926 gal. A 3% annual reduction was achieved in FY 2011, compared with FY 2010 consumption	Continue assessing the fleet and right sizing along with execution of goal 1.9, *"reduce fleet inventory by 35% within the next 3 years relative to a FY2005 baseline."*	L
2.1	13% Scope 3 GHG reduction by FY 2020 (FY 2008 baseline)	FY 2008 Baseline: 23,031 $MTCO_2e$ FY 2011 Actual: 27,728 $MTCO_2e$ FY 2020 Goal: 20,037 $MTCO_2e$	PNNL is initiating steps to increase alternate work locations, install high-end video capabilities in strategic locations to reduce travel, and encourage staff to utilize bus and carpooling for commuting.	M
3.1	15% of existing buildings >5,000 gsf compliant with HPSB Guiding Principles by FY 2015	In FY 2011, 25% of PNNL buildings greater than 5,000 gsf/FIMS are HPSB compliant	PNNL plans to continue trending towards overall goal of 100% of facilities meeting HPSB by FY 2020	L
4.1	26% water intensity reduction by FY 2020 from a FY 2007 baseline	FY 2007 Baseline: 66.88 gal/ft^2 FY 2011 Actual: 31.25 gal/ft^2 FY 2020 Goal: 49.49 gal/ft^2	PNNL plans to continue implementing potable water projects to reduce overall usage as feasible.	L

7.0 Human Resources

7.1 Current and Future Workforce

Over the last 4 years, PNNL has been able to substantially increase the quality of our scientific and technical staff through an integrated capability management process that focuses on strategic hires at all experience levels to fuel strong organizational performance. Driven by our core technical capability needs (Section 3), this process has resulted in a 27% increase in the number of PhD research staff; a doubling of post-doctoral researchers; and a 46.9% increase in students from FY 2009 to FY 2012.

PNNL continually assesses and reviews its staff capabilities through strategic hiring, compensation management, retention efforts, and workforce development. We monitor S&T and M&O staff capabilities throughout the annual planning and budgeting process. As a part of that process, the Executive Committee incorporates strategic hiring targets that align with the PNNL core research capabilities. It has been PNNL's approach to manage thoughtfully our S&T and M&O by focusing on decreasing capacity without losing key staff capabilities. Although it is a challenge as a multiprogram laboratory to manage the ambiguity of federal funding across multiple agencies and sectors, PNNL has processes in place to proactively manage the changing business and budget environment to scale S&T and M&O capabilities either through reductions or re-deployment of staff while mitigating risk.

We have significantly changed the way we attract, develop, retain, and reward our scientific workforce. Promoting recruitment outreach to under-represented populations in Science, Technology, Engineering, and Mathematics (STEM), PNNL continues to evolve its approach to early career recruitment by establishing a Diversity Intern Program office in FY 2012 to leverage our ability to build a diverse workforce pipeline. We are refining our approach to diversity to include a new and strategic focus on sustainability, diversity, and workforce inclusion as an integrated element of the Laboratory's talent management agenda. PNNL continues to invest in outreach and recruitment events at regional and national events supporting diverse women and minority scientists and engineers.

To support the development and career growth of our staff, we have a Corporate University model for training programs that provides interactive learning forums for high potential staff at all levels through the following programs: Advanced Leadership, Emerging Leader, Program Manager Development, Management Skills Development, and the Scientist and Engineer Development. These programs have developed skills for hundreds of staff participants in their specific career paths.

In 2009, the Linus Pauling Distinguished Postdoctoral Fellowship was inaugurated as a part of our ongoing effort to recruit emerging scientific leadership. Up to three Fellows can be selected in a given year, and the appointments are for 3 years. The expectation is that Pauling Fellows will become future scientific leaders at PNNL or elsewhere. There are currently six Fellows with a plan to hire two to three more in 2012. Fellows added in 2011 include:

- Marcel Baer, whose research focuses on developing new research capabilities for simulation of reactivity and structure in complex heterogeneous and homogeneous environments
- Hui Wan, whose research focuses on understanding process interactions in the atmosphere and decreasing the uncertainty associated with component coupling in global climate.
- James Stegen, whose research area focuses on developing ecological models of microbial communities.

Lastly, our joint appointment program continues to strengthen our partnerships with academia, including WSU, the University of Delaware, the University of Utah, and the recent addition of UW (for dual appointments). This program supports strategic scientific hires in the areas of materials, catalysis, computing, chemical imaging and measurement, and data analytics that advance our major initiatives.

7.2 Obstacles and Strategies

Given the challenges we face, it is imperative that PNNL promote its employee experience – the ability to work on technically challenging and nationally important problems; to lead and be recognized in

a field of science; and to work with talented colleagues in an intellectually stimulating environment all while providing a collegial workplace with competitive benefits and compensation.

PNNL fully recognizes the emerging competition for talent in the STEM fields. We believe there are four primary factors worth attention: 1) retirement of baby boomers; 2) smaller talent pools of domestic STEM talent coming out of U.S. universities; 3) evolving foreign financial and academic infrastructures, and 4) a millennial workforce with new expectations of their employers.

We are focused on building an inclusive workforce environment with Life@PNNL and its approach to diversity, creating an even more flexible working environment. We are implementing market-based career series that enable increased visibility to career paths and accelerated talent management activities. PNNL is focused on using these efforts to enhance the employee experience for all generations of workers.

The Laboratory has identified management and operations major initiatives to enable the effective and efficient conduct of research, as described below.

Winning the Competition for Talent. To accomplish its mission, PNNL must attract and retain the best and brightest minds from around the world, and we pride ourselves on a workforce that includes a diverse set of outstanding scientists, professionals, and support personnel dedicated to scientific discovery and finding solutions to challenges of national and international importance. PNNL's leadership continues to review talent and organizational readiness to respond to the complex needs of the Laboratory. While FY 2012 budget uncertainties may result in a reduction of full-time equivalents (FTEs), we remain committed to developing the workforce needed to advance our scientific vision. Four areas of focus for FY 2012 include defining and communicating a clear direction for the future and creating organizational alignment with the Institutional strategy and major initiatives; enabling staff at all levels to lead and influence across multiple groups and constituencies; effectively managing talent to ensure mission ready core technical capabilities; and ensuring strong business and operational performance.

Productivity in a Global, Virtual World. Scientific and technological research is a global enterprise and our success depends on enabling all staff to be fully productive in this global – and increasingly virtual – world, in a way that is environmentally sustainable. Our efforts are focused on enabling our staff to work productively where they want to work and live by:

- piloting and implementing tools, policies, practices, and procedures that fully support and enable flexible work practices that attract and enable multi-generational staff by managing outcomes, not presence. PNNL will continue to expand this footprint of virtual capabilities in FY 2012 and beyond, thusly shifting the culture significantly and redefining "how" we work with less reliance on "where" we work.
- lowering the Laboratory's environmental footprint while increasing staff satisfaction with their working environment.

STEM Education. As a direct response to the national concern over the lack of students entering the STEM disciplines, the Strengthen and Advance STEM Education Initiative is impacting the educational ecosystem by focusing on the preparation of today's students for tomorrow's world. It spans everything from sowing the seeds of wonder and inquiry among our school children to providing rich, hands-on learning experiences for educators and potential PNNL employees. Because the STEM disciplines are critical to our nation's ability to compete globally and to PNNL's ability to transform the world through courageous discovery and innovation, we are strengthening and advancing STEM Education by:

- positively impacting 9–12 STEM education through the innovative Delta High School Partnership
- mobilizing the power of a national laboratory to cultivate rich classroom learning environments through PNNL's impact on the LASER partnership's leadership initiatives
- connecting our STEM initiative to Battelle's leadership efforts, aligning our student programs to new DOE workforce development goals, and seeking additional opportunities to collaborate with key STEM education advocates and stakeholders through collaborations with Battelle, DOE, and others.

8.0 Cost of Doing Business

8.1 Overhead Budget Process

The Laboratory's integrated annual planning process is jointly stewarded by the Chief Financial Officer, the Deputy Director for Science and Technology, and the Chief Operations Officer. Overhead expenses are in one of four portfolios: research, management and operations, facilities and infrastructure, and fixed costs. Each portfolio budgets for core activities and strategic initiatives. Final decisions for institutional and organizational overhead budgets are made by PNNL's Executive Committee.

The planning process begins with consideration of strategic initiatives based on alignment to strategy. Formal project management methods are used to track performance and measure investment impact. Requests for resources for core activities are evaluated against a cost-model or standard for that portfolio, evaluated for strategic alignment, and prioritized against available resources. The total overhead budget is sized to maintain fully burdened charge-out rates (CORs) at escalation rates consistent with established goals.

Since FY 2007, PNNL's Executive Committee has maintained a goal to limit the annual average escalation on burdened CORs to 4.2%, below the 10-year average of 4.8%. This was initially done to accommodate the overhead resources necessary to keep core capabilities mission ready through completion of the CRL and 300 Area facility life extension projects. This limit has been maintained to fund additional strategic investments in facilities and infrastructure, institutional computing, and management and operations. Aggressive cost management over the years has resulted in a cumulative burdened COR increase of 3.4% (Figure 3).

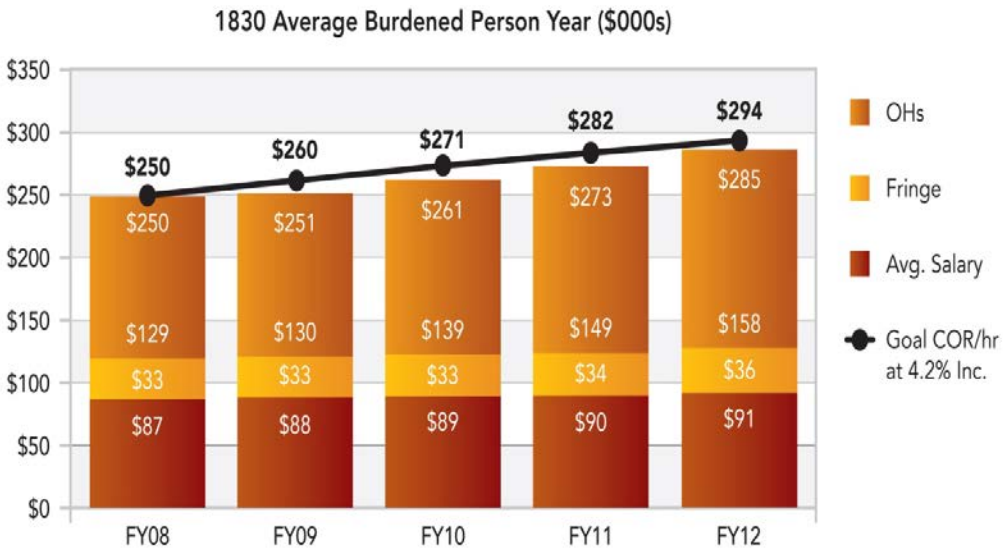


Figure 3. 1830 Average Burdened Charge-Out Rates

The FY 2011 increases in the percentages for "Total Overhead/Total Laboratory Costs" and "Total Overhead/Total Laboratory Operating Costs" shown in Table 6 below are a result of increased LDRD investment in our core technical capabilities (described in more detail below) and increased investments to modernize our facilities and infrastructure (described in detail in Section 6). It is important to note that this increased investment to keep our capabilities mission-ready was accomplished while staying well below the average charge out rate goal set by management (3.4% actual vs. a 4.2% goal; Figure 3). In addition, the Laboratory is experiencing a large drop in business volume in FY 2012, which is expected to continue into FY 2013 (lab costs dropping from $1.1B in FY 2011 to $921M expected in FY 2013). This has a negative impact on many of the metrics in Table 6. FY 2013 planning is being performed with the expectation of improving many of these metrics. For example, indirect FTEs are being studied to determine what reductions are necessary to recover a 58% Direct FTE Ratio.

Table 6. Laboratory Overhead Trends
(cost data in $M; data provided represents the total consolidated laboratory)

	FY 2009	FY 2010	FY 2011	FY 2012 est.	FY 2013 est.
1. Direct FTE Ratio					
Numerator: Direct FTEs,[a] which represent time charged to client funded work, [b] including capital but excluding LDRD	2226	2405	2411	2270	2202
Supplemental Data: Indirect FTEs (all non- direct FTEs, to include LDRD and organizational burden[c])	1631	1698	1769	1710	1592
Denominator: Total FTEs (subtotal of direct and indirect FTEs)	3857	4103	4180	3980	3794
Direct FTE Ratio (%): Direct FTEs/Total FTEs	57.7%	58.6%	57.7%	57.0%	58.0%
2a. Total Overhead/Total Laboratory Cost					
Numerator: Total overhead cost; includes institutional overhead, LDRD, and organizational burden[c] to the extent this overhead is allocated to client-funded work[b]	303.3	338.0	366.8	361.7	325.5
Denominator: Total laboratory cost includes all cost charged to client funded work[b] (operating and capital). Includes subcontracts and procurements[d] and line item construction costs.	1058.6	1112.4	1105.5	1007.6	921.3
Total Overhead/Total Laboratory Cost (%)	28.7%	30.4%	33.2%	35.9%	35.3%
2b. Total Overhead/Total Laboratory Operating Cost					
Numerator: Same as preceding metric	303.3	338.0	366.8	361.7	325.5
Denominator: Same as preceding metric, excluding line item construction costs	959.6	1055.9	1099.1	1007.6	921.3
Total Overhead/Total Laboratory Operating Cost (%)	31.6%	32.0%	33.4%†	35.9%	35.3%
2c. Total Overhead/Total Internal Laboratory Operating Cost					
Numerator: Same as preceding metric.	303.3	338.0	366.8	361.7	325.5
Denominator: Same as preceding metric, exclude sub-contracts/ procurements[d] charged to client funded work.[b]	645.8	709.2	753.2	688.4	629.5
Total Overhead/Total Internal Laboratory Operating Cost (%)	47.0%	47.7%	48.7%	52.5%	51.7%
3. Fringe Rate					
Numerator: Total cost of employee benefits (including statutory benefits), not including paid absences	141.1	147.6	150.7	159.2	143.1
Denominator: Total base salary cost	363.9	400.3	418.5	416.5	408.9
Fringe Rate (%)	38.8%	36.9%	36.0%	38.2%	35.0%
4. Labor Multiplier on a DOE Operating Funded Project*					
Base Salary of $100K: Includes leave/absence costs.	$100K	$100K	$100K	$100K	
Fully Burdened Salary Cost: Multiply $100K base salary by fringe benefit (excluding leave), overhead (use an average for all scientific divisions), G&A, LDRD, IGPP/IGPE, fee, and etcetera, rates based on your laboratory's burdening methodology for a DOE operating funded project. *Do not include composite rates, such as special rates for large construction projects.* Use final indirect rates for FY 2009, FY 2010, and FY 2011, current forward pricing rates for FY 2012, and do not provide a projection for FY 2013. When complete, this calculation will equal the same number used in the Budget Officers' Conference Metrics Section 3.a "Burdened Labor (DOE)." Please be sure to confirm data with the laboratory budget officer.	287.1	293.6	296.2	305.6	
Labor Multiplier: Divide fully burdened salary cost by $100.0K	2.87	2.94	2.96	3.06	

Notes: FY 2009, FY 2010, and FY 2011 data reflect actual costs. FY 2012 and FY 2013 are estimates (adjusted for escalation). Cost data includes Use Permit activity.
[a] An FTE is calculated as actual hours charged divided by the expected hours to be charged by a normal employee during a year..
[b] "Client funded work" refers to "direct charges"/"direct funded work."
[c] "Organizational burden" refers to an overhead pool that accumulates the cost of managing and operating an organization or group of organizations and is usually allocated on a rate established specifically for recovering the cost of the organization and/or grouping. It includes space charges.
[d] "Subcontracts and procurements" include services performed for and purchases made by the laboratory that are charged directly to programmatic work (*e.g.*, subcontracts for consulting, postdoctoral R&D fellowships at national laboratories, construction, architect and engineering services, material and equipment purchases, inter-entity work orders to other DOE laboratories, R&D at universities, etc.).
* Do not provide FY 2013 projected data for item 4. Labor Multiplier.
† ARRA Smart Grid project is 1831.

8.2 Cost Drivers and Management/Mitigation Strategies

PNNL has successfully managed several significant cost challenges while avoiding significant indirect rate increases through effective cost management, and operational efficiencies.

Employee Pension Costs. We have been proactive in managing the PNNL pension plan to mitigate the impact of increasing pension contributions by implementing significant plan amendments and building up "credit balances." Through FY 2011, PNNL has established credit balances of $44M, which will reduce funding requirements in FYs 2012–2015, thereby mitigating the impact of required funding peaks that occur during potentially reduced budget years. In FY 2009, Battelle made a significant amendment to the plan with a combined savings of $70–$80M over 10 years, and an additional amendment is being implemented effective July 1, 2012, which will initially reduce annual contributions by $15M, increasing to $20M by FY 2018.

Cost of Site Services. PNNL purchases a number of critical services from the existing Hanford Site service contractors. PNNL is working closely with PNSO to determine the Laboratory's long-term needs for support services and the best competitive source of those services. A comprehensive approach has been developed that includes both purchasing services from the Hanford Site and proposals for third-party sources to provide the best value for DOE-SC and PNNL. As a result, PNNL will be subcontracting with a third-party to provide occupational medical services, which saves money and improves services, and is pursuing with PNSO and DOE-RL the provision of electrical power services by the City of Richland to the 300 Area as well as having the City of Richland provide fire protection and emergency response services, which will result in significant cost savings for PNNL and the Government.

8.3 Decisions and Trade-Offs

The Laboratory has a limited amount of discretionary resources available for investment. As a result of our cost control efforts, we have been able to focus our overhead resources to advance the Laboratory's scientific vision and strategy. Based on our strategic prioritization, we significantly increased (nearly 50% over the past 4 years) the LDRD resources invested in our core capabilities and major initiatives, increased our spending on strategic facilities and infrastructure, and provided a significant new investment in PNNL's institutional computing capability all while reducing our overhead costs for management and operations through increased efficiency.

Our FY 2012 science and technology investment portfolio includes investments in chemical imaging, the grid, detecting complex threat signatures, aerosol physics and chemistry, coupling earth and energy systems regional modeling and integrated assessment, transformational chemical and materials synthesis for energy conversions and storage, novel architectures and algorithms for extreme-scale computing, and understanding microbial communities. At the same time, we also make investments in our facilities and infrastructure and management and operations, all focused on significantly increasing the efficient and effective conduct of research. The two largest investments in FY 2012 are:

Integrated Management Systems (IMS) Improvement Project. The PNNL IMS Improvement Project is a multiyear investment to integrate people, processes, and information systems and reduce system complexity in order to increase efficiency and reduce staff frustration. Over 3–5 years, PNNL will significantly reduce the total number of information systems and increase our ability to respond to required business changes. The new systems will enhance integrated capability management while reducing the Laboratory's overall cost of doing business.

Facilities and Infrastructure. PNNL is committed to keeping our core technical capabilities fully mission ready. Through aggressive cost management, PNNL has made strategic investments to optimize current facilities and provide new, modern laboratory facilities to enable scientific excellence. (See Section 6 for details.) As a result, annual capital investments (through IGPP) on the PNNL campus have more than tripled since FY 2008.

Appendix 1 Annual Work for Others Plan

This appendix describes the work PNNL performs for government agencies, including DoD, NRC, DHHS, NASA, EPA, the U.S. Department of the Treasury, the U.S. Department of State, and other federal and non-federal agencies, as well as the DHS.

U.S. Department of Defense

PNNL's work for DoD clients enhances the Laboratory's science and technology capabilities that advance DOE missions in scientific discovery and innovation, energy, environment, and national security. Primary clients include Joint Improvised Explosive Device Defeat Organization, Air Force Research Laboratory, Office of Naval Research, Army Research Laboratory, U.S. Army Research and Development Command, U.S. Army Corps of Engineers, DARPA, and the Defense Threat Reduction Agency. The DoD research portfolio provides basic science solutions to extremely difficult national needs that support both DOE's and DHS's missions in national security, energy security, environment management and homeland security. More specifically, PNNL is developing:

- **Signature discovery and the development of novel detection systems** for CBRNE threats that benefit both NNSA and DHS programs.
- **Durable and portable energy sources** with immediate applications for soldier portable systems and unmanned underwater vehicles that benefit BES and EERE programs.
- **Synthesis of self assembled materials** designed to capture CO_2 that benefit DOE's FE program
- **Energy systems management** for buildings, vehicles, and smart grid analysis, design, and operation that benefit DOE's EERE, OE, and FE programs.
- **New or improved methods of tagging, tracking, and locating** using RFID's for logistic control and asset health monitoring which benefits both NNSA and DHS programs.
- **Environmental characterization and remediation technologies** to balance environmental recovery and restoration, power generation, and local water use with benefit to EERE and EM programs.
- **Design and fabrication of sensors** for monitoring the health of tactical assets that benefit both NNSA and DHS programs
- **Cyber security software** for critical infrastructure protection and operational support that benefit NNSA and EERE programs and also DHS programs.

The basic and applied research programs funded by DoD leverage, strengthen, and enhance PNNL's core capabilities in chemical and molecular sciences, biological systems science, subsurface science, applied nuclear science and technology, applied materials science and engineering, chemical engineering, systems engineering and integration, and advanced computer science, visualization and data. As a result of PNNL's capabilities and decades of experience in signature discovery and detection for DOE and DoD, the Laboratory continues to lead a cooperative program with the DHS to address the detection and defeat of person-borne and vehicle-borne improvised explosive devices.

PNNL expects flat funding in the out years with continued demand for our expertise in energy systems and materials applied to fuel cell technologies and advanced nuclear, chemical, and biological sensor technologies to detect weapons of mass effect.

U.S. Nuclear Regulatory Commission

PNNL provides expertise to NRC supporting their nuclear safety mission. Because of our domain knowledge in nuclear reactor technologies, NRC research programs address nuclear fuels, nuclear reactor pressure boundary materials, nuclear materials characterization, environmental transport of radionuclides, decommissioning studies, emergency preparedness, spent fuel storage, nuclear waste handling, nuclear

reactor design reviews and license extensions, nuclear facility safety, new reactor siting, and regulatory criteria development. PNNL provides this expertise to the following NRC offices:

- **Office of New Reactors**: PNNL supports design certifications, environmental reviews, and engineering and scientific support in various technical areas of reactor operation and nuclear safety.
- **Office of Nuclear Reactor Regulation**: PNNL provides technical reviews of in-service inspection relief requests, development of regulatory requirements for nuclear plant fire protection programs, safety and analysis in the area of commercial in-reactor fuel performance, and multidisciplinary managerial and technical expertise to assist licensing reviews.
- **Office of Nuclear Regulatory Research**: PNNL provides expertise in nondestructive evaluation of reactor vessel materials and nuclear fuel performance assessments, environmental fate and transport, and biosphere modeling for food chain radionuclide uptake pathways.
- **Office of Nuclear Materials Safety and Safeguards**: PNNL assists in implementing domestic and international safeguards policy and regulation for fuel cycle facilities, including material control and accountability.
- **Office of Nuclear Security and Incident Response**: PNNL develops radiological consequence assessment tools and train staff for such events and develops methods and regulatory guidance to improving cyber security preparedness at operating power plants.
- **Office of Federal and State, Materials and Environmental Management**: PNNL provides technical expertise to the NRC for the licensing of uranium recovery operations.

PNNL's work for the NRC supports the continued operation of 104 nuclear plants, which provide approximately 20 percent of the nation's electricity, as well as support for new reactor licensing reviews. In addition, the newly established Japan Lessons-Learned Project Directorate within the Office of Nuclear Reactor Regulation, charged with implementing regulatory actions prompted by the accident at Fukushima, will greatly benefit from PNNL's technical resources. The Laboratory's NRC business, which is largely driven by environmental reviews and materials science research, is expected to remain steady in the out years.

The NRC programs build on and strengthen PNNL's core capabilities in advanced nuclear science and technology, subsurface science, advanced material science and engineering, systems engineering and integration, and advanced computer science, visualization and data. The research activities of these programs complement DOE's NE, EM, and NNSA programs in nuclear energy, environmental cleanup, and nuclear nonproliferation. Collectively, they advance DOE and DHS missions in scientific discovery and innovation, energy security, environmental management, national security, and homeland security.

U.S. Department of Health and Human Services

PNNL has several programs funded by the NIH, including programs with the National Institute of General Medical Sciences; the National Institute of Allergy and Infectious Diseases; the National Institute of Diabetes, Digestive, and Kidney Diseases; the National Cancer Institute; and the National Institute of Environmental Health Sciences. These NIH funded programs, described below in detail, augment facilities and equipment available at PNNL to serve DOE programs within the SC-BER for life science research, EM relative to environmental health and risk, and NNSA relative to radiation exposure. PNNL performs research for the following NIH offices:

- **National Institute of General Medical Sciences**: PNNL is establishing the *Proteomics Research Resource for Integrative Biology* as a national resource for scientists across the country and developing *Advanced Proteomic Instrumentation* enabling high-sensitivity measurements of small, nonconventional proteomic samples for studying large and complex protein sets.
- **National Institute of Allergy and Infectious Diseases**: PNNL leads a multi-institutional collaboration as the *National Center for the Systems Biology of Enteric Pathogens* for where

proteomic technologies developed at PNNL are applied to understanding the mechanism of virulence used by enteric pathogens; serves as a resource for both proteomics and computational systems biology for the *Pacific Northwest Regional Center of Excellence* focused on the response of a host to viral infections with emphasis on the effects of aging on the immune response to infection; and is developing *Medical Countermeasures for Radiation Exposure* using natural-materials- and nano-materials-based decorporation agents that could be used to mitigate the effects of radiological attack.

- **National Institute of Diabetes, Digestive, and Kidney Diseases**: PNNL is defining the sample processing and liquid chromatography separation conditions necessary for developing technological approaches and providing a basis for high-throughput studies of large numbers of samples, leading to identification of potential biomarkers for pre-diabetes and types 1 and 2 diabetes, as well as potential biomarkers predictive of impending diabetic complications.
- **National Cancer Institute**: PNNL is conducting research to identify protein biomarkers in blood plasma that may be used in the *Early Detection of Cancer* in breast, prostate, and other glands; developing a *Cancer Chip* using PNNL's yeast surface display of single-chain antibodies; and developing *Next-Generation Proteomic Platforms* using ion mobility separation technologies to provide the measurement throughput required for clinical applications.
- **National Institute of Environmental Health Sciences**: PNNL's expertise in systems toxicology, imaging, and proteomics led to establishing a *Center for Novel Biomarkers of Response* to study the response to inhaled particulates using animal models and human patients.

A combination of PNNL's core capabilities form the basis of the expertise used in this portfolio of NIH-funded research projects, including biological systems science, chemical and molecular sciences, applied nuclear science and technology, subsurface science, and advanced computer science, visualization and data. Out year funding is expected to remain flat (or decline slightly) for the current portfolio focused in the areas of microbial pathogenesis and structural biology of proteins involved in pathogenesis, health effects of nanoparticles, medical countermeasures to radiation exposure, biomedical computing, and disease biomarker research. The work funded by NIH builds on and strengthens PNNL's core capabilities while also advancing DOE's missions in scientific discovery and innovation and national security.

Other Federal Agencies

PNNL performs R&D for several federal agencies that include Department of Treasury, Department of State, EPA, and NASA. The portfolio of work for these agencies is described below.

U.S. Department of Treasury's Internal Revenue Service

PNNL continues to provide the law enforcement community with unique or specialized analytical capabilities and investigative support tools and techniques. PNNL draws upon its core capabilities in chemical and molecular sciences, and advanced computer science, visualization and data to identify diesel fuel that has been fraudulently categorized or altered to appear to be a nontaxable material. The results provide sufficient evidence for the U.S. Department of Treasury's Internal Revenue Service to thwart illicit activities designed to avoid the payment of excise taxes. PNNL has developed a strong capability in chemical analysis based on extensive work conducted on behalf of the DOE-SC. The U.S. Department of Treasury benefits from this expertise while PNNL further develops our core capabilities (mentioned above) for ongoing and related programs within SC and NNSA while also advancing DOE's missions in scientific discovery and innovation and national security.

U.S. Environmental Protection Agency

PNNL conducts research to support the EPA in the development, implementation, and enforcement of environmental regulations. This research includes contaminant or hazardous waste fate and transport in soil and water (fresh and marine), air, and biota. The Laboratory is also developing human health risk

assessment information, methods, and guidance, while improving the science and technology associated with risk assessment. In addition, PNNL is developing innovative compliance information tools for government and industry. These programs benefit DOE's programs in SC-BER, FE, EM, EERE, and NNSA. EPA programs leverage and strengthen PNNL's core capabilities in environmental subsurface science, climate change science, advanced nuclear science and technology, systems engineering and integration, and advanced computer science, visualization and data. EPA-funded programs at PNNL advance DOE's energy security, environmental management, and national security missions.

U.S. Department of State

The U.S. Department of State primarily relies on PNNL's core capabilities in advanced nuclear science and technology, systems engineering and integration, and computer science, visualization and data to conduct international nuclear nonproliferation work in cooperation with NNSA. PNNL designs, develops, and deploys advanced sensing, measurement, and evaluation technologies for international safeguards and nuclear safety systems and trains international border and law enforcement personnel to interdict weapons of mass destruction. This work expands PNNL's knowledge of CBRNE threats faced by the United States and the world. It strengthens PNNL's core capabilities mentioned above and advances DOE's and DHS's missions in nuclear nonproliferation and homeland security.

National Aeronautics and Space Administration

PNNL provides NASA with expertise in energy and environmental technologies, climate physics, and space radiobiology. PNNL's portfolio of NASA funded programs has strong synergies with DOE funded programs in SC-BER. The primary research and development areas involve atmospheric and climate change modeling; basin, watershed, and coastal assessment; regional impacts of bioenergy production; and nuclear safety and cellular radiation science. This work builds and strengthens PNNL's core capabilities in climate change science, subsurface science, nuclear science and technology, and biological systems science and advance DOE's missions in scientific discovery and innovation, energy security, and environmental management.

Other Government Agencies

PNNL performs work for other government agencies that include the General Services Administration, Library of Congress, and NOAA. PNNL also provides expertise in nuclear fuel cycle, non-nuclear energy security, and information operations of intelligence interests to several government agencies that conduct classified activities for all-source intelligence analyses, scientific investigations, and innovative technologies for critical national security challenges. The collective portfolio of work can be broadly described as follows:

- **CBRNE threat detection systems and technologies** for various environments; nuclear nonproliferation training for border enforcement personnel, including marine environments, dosimetry to support the National Voluntary Laboratory Accreditation Program; information analytics; and data visualization tools and systems, including INSPIRE, cyber security for critical infrastructure protection, and multithreaded architectures.
- **Systems modeling, engineering, and processing** include nondestructive testing and imaging systems; environmental fate and transport analysis for radiological and non-radiological contaminants; climate change and atmospheric measurements as a function of primary anthropogenic investigations; process engineering for biofuel production; and energy efficiency in buildings..

These programs strengthen PNNL core capabilities in advanced computer science, visualization, and data; applied nuclear science and technology; biological systems science; chemical engineering, systems engineering and integration; and environmental subsurface science. Collectively, these programs also

advance DOE's missions in scientific discovery and innovation, energy security, environmental management, national security, and homeland security.

PNNL's funding profile in this category is driven predominantly by the Special Programs sector for research in the areas of cyber security intelligence analysis, measurement and signature intelligence research, human information and interaction tools, and information operations applied to the intelligence community needs. Due to the recent fiscal climate and budgetary projections, PNNL is projecting a decline in funding within the Special Programs sector in FY 2012 and FY 2013.

Non-federal Agencies

PNNL conducts work for state and local governments and for private organizations that conduct work funded by government agencies. PNNL performs research for the State of Washington and King County to solve critical environmental and natural resource problems for local highway systems and the Puget Sound area. The Laboratory also provides energy and environmental technology expertise to the California Institute of Energy and Environment and California Energy Commission.

Collectively, the Laboratory's research portfolio for non-federal agencies can be described as follows:

- **Smart grid operations**: scientific forecasting for capacity and ramping and operational impacts of wind and solar generation.
- **Cyber security**: energy smart data centers for data-intensive computing applications.
- **BWR MOX Fuel**: development of fuel design for irradiation
- **Majorana Project**: design of a Tonne-scale germanium detector for neutrinoless double-beta decay
- **Solid-oxide fuel cell**: for powering unmanned underwater vehicles
- **Climate research**: and its impacts at a regional scale
- **Biomedical research**: internal dose calculations in support of clinical trials for cancer research.
- **Therapeutic protein targets**: human metabolic diseases.
- **Radioactive source materials**: preparation and storage of targets.

These programs leverage and strengthen PNNL's core capabilities in biological system sciences, subsurface science, advance nuclear science and technology, chemical and molecular sciences, systems engineering and integration, and advanced computer science, visualization, and data. These programs strengthen the science and technology programs for NNSA, EM, BER, and SC, advancing DOE's and DHS's missions in scientific discovery and innovation, energy security, environmental management, national security, and homeland security. PNNL expects funding growth in the out years due to demand for the Laboratory's expertise in applied nuclear science and technology to address both fuel design for commercial reactors and the emerging S&T needs due to the Fukushima crisis in Japan. In addition, a significant portion of work currently begin performed under the Use Permit will transition to Non-Federal Work For Others resulting in increased out-years sales projections

Department of Homeland Security

The DHS was created to prevent and deter terrorist attacks within the United States and reduce the nation's vulnerability to terrorism. Its charter also includes preparation for and response to all hazards, including natural disasters. PNNL provides DHS with critical scientific and technological resources to enable federal, state, and local officials to counter terrorist threats and respond to national emergencies.

PNNL stewards an extensive portfolio of projects supporting DHS, covering all phases of innovation—research and development, engineering, testing, deployment, training, and operations. The Laboratory has developed a deep understanding of the regional emergency management needs that enable Laboratory staff to develop, test, and deploy new approaches and solutions targeted to the end user community.

PNNL performs research and development for DHS in chemical and biological sciences, information analytics, cyber security, radiation and nuclear detection, explosives detection, systems engineering, and maritime security. This portfolio of work has strong synergies with DOE missions and programs, and collectively advances DOE's missions in scientific discovery and innovation and national security. Details for each research area are provided below.

Chemical and Biological Sciences

PNNL supports DHS efforts to increase the nation's preparedness against chemical and biological threats with work in chemical and biological forensics, developing and evaluating new assays, teaming with stakeholders to create protocols and procedures for detection and analysis, and developing new tools to help emergency managers make sound decisions during chemical and biological events. The Laboratory's breadth and depth of experience in microbiology, analytical chemistry, statistics and analytics enables research teams to develop chemical and biological forensics procedures, which are essential to DHS. PNNL's portfolio of research in chemical and biological sciences includes:

- Discovery and development of chemical and biological signatures associated with threats
- Multidisciplinary approaches to develop new methods, techniques, and processes to collect, separate, concentrate, and analyze field samples for forensic attribution
- Recovery and restoration of critical infrastructure following the release of a biological agent.

This work strengthens the Laboratory's core capabilities in chemical and molecular sciences, biological systems science, applied materials science and engineering, applied nuclear science and technology, and systems engineering and integration. This work supports DOE programs in SC-BER and NNAS, and advances DOE's mission in scientific discovery and innovation and national security.

Information Analytics

Most DHS operational components and state and local agencies must integrate and analyze large amounts of disparate, conflicting, and dynamic information from multiple, and sometimes incompatible, sources to identify and prevent emerging threats, protect the nation's borders, and respond to natural, accidental, and intentional disasters.

PNNL is making scientific and technical advances in the field, partnering with universities and industry, and transitioning technologies to solve operational component and end user key needs for information analysis. PNNL's support in this area includes:

- Leadership in visualization and analytics
- Precision information environments that combine physical models, real-time data streams, and other information to support actions, assessments, and decision-making in emergences
- Wide area surveillance and change detection analytics for protecting critical infrastructure
- Develop and deploy robust analytical tools for law enforcement and intelligence analysts
- Technologies and platforms for regional information sharing and collaboration amongst first responders and emergency management community.

This work strengthens the Laboratory's core capabilities in advanced computer science, visualization, and data and supports DOE's programs within NNSA and IN while advancing DOE's missions in national security and scientific discovery and innovation.

Radiation and Nuclear Detection

The government has made significant investments to detect and prevent the illicit transport of radiological and nuclear materials into the United States, yet vulnerabilities exist and new approaches are needed. PNNL has extensive experience in radiological and nuclear science, radiochemistry, nuclear

engineering, health physics, and dosimetry and engineered systems that continue to be leveraged to meet DHS mission requirements. The Laboratory's unique combination of technical expertise, independence, and deep understanding of the operational environment allows PNNL to contribute to the variety of challenges DHS faces. Our portfolio of work in support of DHS includes:

- Leadership of the Radiation Portal Monitor Project for the Domestic Nuclear Detection Office (DNDO), providing comprehensive scientific and technical services to interdict realistic radiological and nuclear threats at our borders
- Stand-up the Rail Test Center to test and evaluate radiation detection systems in an intermodal rail environment
- Develop new signatures associated with illicit nuclear trafficking and strategies for the Global Nuclear Detection Architecture
- Information driven approach to develop new semiconductor materials for gamma detection
- Development of new analytical methods to improve the speed, accuracy, precision and sensitivity of isotopic ratio measurements.

This work strengthens PNNL's core capabilities in advanced nuclear science and technology, systems engineering and integration, and advanced computer science, visualization, and data, while supporting DOE's NNSA programs. Furthermore, these efforts advance DOE's missions in national security and scientific discovery and innovation.

Cyber Security

Working with customers like the National Cyber Security Division's U.S. Computer Emergency Response Team and the DHS Science and Technology Division, PNNL is helping to secure some of the nation's most critical information infrastructure. PNNL is applying its nationally recognized visualization and analytic techniques against cyber security large-data analytic challenges. PNNL's cyber research for DHS includes:

- Develop, integrate and deploy computer network traffic analysis technology US-CERT
- Provide a dynamic multi-user controls systems research laboratory that combines virtual, simulation, and physical environments.

These programs build on and strengthen PNNL's capability in advanced computer science, visualization, and data; systems engineering and integration; and advancing DOE's mission in national security.

Explosives Detection

PNNL's capabilities and experience support research and development efforts in infrastructure protection and explosives detection for various DHS components. The Laboratory's multidisciplinary approach to the detection of explosives combines chemical and molecular detection with multimodal imaging and information analytics. PNNL knowledge and expertise in this area is sought by DHS to review related programs and strategies for key technical areas. PNNL's portfolio of work in support of DHS missions include:

- Leadership of a multi-laboratory consortium to bring the expertise of the entire DOE national laboratory complex to bear on the detection of explosives.
- Development of signatures associated with person- and vehicle-borne improvised explosive devices
- Exploit data from multi-sensor systems and increase probability of detection while simultaneously reducing false alarms
- Non-invasive technologies for screening cargo and large containers at various locations.

This work strengthens the Laboratory's core capabilities in chemical and molecular sciences, chemical engineering, applied materials science and engineering, computer science, visualization and data, and

systems engineering and integration. These programs advance DOE's missions in scientific discovery and innovation and national security.

Systems Engineering

Increasingly, homeland security challenges cross threats, organizations, and jurisdictions, making it vital that homeland security agencies employ robust systems engineering practices. PNNL is using its experience and expertise to help DHS effectively involve stakeholders from federal, state, local, and private organizations to develop, test, evaluate, and deploy technologies that address these challenges. PNNL is known for its systems engineering capabilities and for leading large demonstration and deployment projects. PNNL's work for the DHS includes:

- Leadership of the Radiation Portal Monitoring Projects for DNDO to coordinate the evaluation, procurement, and installation of over 1,500 systems nationwide
- Developed and deployed a wide area surveillance system at Boston's Logan International Airport, in collaboration with MIT, to improve aviation security.
- Developed and demonstrated, in partnership with ILC Dover and West Virginia University, an emergency inflatable plug design to seal off mass transit tunnels rapidly in the event of natural or man-made disaster.

This work strengthens the Laboratory's core capabilities in systems engineering and integration. These programs advance DOE's mission in national security.

Maritime Security

The maritime system is critical for the sustained economy of the United States. PNNL is developing and deploying tools and technologies to improve the security of our nation's coastline and waters while maintaining the flow of commerce and protecting travelers. PNNL's extensive experience in developing and deploying scientific and technological solutions allows the Laboratory to address maritime security through

- Collecting, processing, analyzing, and integrating information and data associated with illicit trafficking across the maritime domain
- Developing composite signatures using several sensor modalities the same maritime environment to differentiate between hazardous and benign activities and materials
- Training state and local authorities on ways to deploy radiation and nuclear detectors on small vessels
- Analyzing environmental and biological factors such as in aquatic environments.

This work strengthens the Laboratory's core capabilities in systems engineering and integration and supports DOE's NNSA programs. These efforts advance DOE's missions in scientific discovery and innovation and national security.

In addition to the capabilities and programs described above, PNNL also conducts programs for DHS that engage regional partners through the Northwest Regional Technology Center for Homeland Security, which serves as a model for bringing together state, local, tribal, private sector, and regional agencies and jurisdictions involved in all aspects of homeland security and helps build regional resilience. PNNL also works with the DHS Office of University Programs and academic institutions around the country to apply science to solving homeland security problems.

PNNL expects stable funding from DHS over the next few fiscal years. As the Radiation Portal Monitor Project transitions from building out the network to sustaining the network, PNNL expects reduced funding for this project. However, we expect the combination of our unique technical capabilities and deep understanding of the DHS mission space to result in new programs with DHS S&T and other components to make up the difference.

Appendix 2 Mission Relevance of Core Capabilities

Scientific Discovery and Innovation (SC)

ASCR

1. To develop mathematical descriptions, models, methods, and algorithms to accurately describe and understand the behavior of complex systems involving processes that span vastly different time and/or length scales.
2. To develop the underlying understanding and software to make effective use of computers at extreme scales.
3. To transform extreme scale data from experiments and simulations into scientific insight.
4. To advance key areas of computational science and discovery that further advance the missions of the SC through mutually beneficial partnerships.
5. To deliver the forefront computational and networking capabilities to extend the frontiers of science.
6. To develop networking and collaboration tools and facilities that enable scientists worldwide to work together.

BES

7. Discover and design new materials and molecular assemblies with novel structures, functions, and properties, and to create a new paradigm for the deterministic design of materials through achievement of atom-by-atom and molecule-by-molecule control.
8. Conceptualize, calculate, and predict processes underlying physical and chemical transformations, tackling challenging real-world systems – for example, materials with many atomic constituents, with complex architectures, or that contain defects; systems that exhibit correlated emergent behavior; systems that are far from equilibrium; and chemistry in complex heterogeneous environments such as those occurring in combustion or the subsurface.
9. Probe, understand, and control the interactions of phonons, photons, electrons, and ions with matter to direct and control energy flow in materials and chemical systems.
10. Conceive, plan, design, construct, and operate scientific user facilities to probe the most fundamental electronic and atomic properties of materials at extreme limits of time, space, and energy resolution through x-ray, neutron, and electron beam scattering and through coherent x-ray scattering. Properties of anticipated new x-ray sources include the ability to reach to the frontier of ultrafast timescales of electron motion around an atom, the spatial scale of the atomic bond, and the energy scale of the bond that holds electrons in correlated motion with near neighbors.
11. Foster integration of the basic research conducted in the program with research in NNSA and the DOE technology programs, the latter particularly in areas addressed by Basic Research Needs workshops supported by BES in the areas of the hydrogen economy, solar energy utilization, superconductivity, solid-state lighting, advanced nuclear energy systems, combustion of 21st century transportation fuels, electrical-energy storage, geosciences as it relates to the storage of energy wastes (the long-term storage of both nuclear waste and carbon dioxide), materials under extreme environments, and catalysis for energy applications.

BER

12. Obtain new molecular-level insight into the functioning and regulation of plants, microbes, and biological communities to provide the science base for cost-effective production of next generation biofuels as a major secure national energy resource.

13. Understand the relationships between climate change and Earth's ecosystems, develop and assess options for carbon sequestration, and provide science to underpin a fully predictive understanding of the complex Earth system and the potential impacts of climate change on ecosystems.
14. Understand the molecular behavior of contaminants in subsurface environments, enabling prediction of their fate and transport in support of long term environmental stewardship and development of new, science-based remediation strategies Understanding the role that biogeochemical processes play in controlling the cycling and mobility of materials in the subsurface and across key surface-subsurface interfaces in the environment enabling the prediction of their fate and transport.
15. Make fundamental discoveries at the interface of biology and physics by developing and using new, enabling technologies and resources for DOE's needs in climate, bioenergy, and subsurface science.
16. Operate scientific user facilities that provide high-throughput genomic sequencing and analysis; provide experimental and computational resources for the environmental molecular sciences; and resolve critical uncertainties about the role of clouds and aerosols in the prediction of climatic process.

FES

17. Advance the fundamental science of magnetically confined plasmas to develop the predictive capability needed for a sustainable fusion energy source.
18. Support the development of the scientific understanding required to design and deploy the materials needed to support a burning plasma environment.
19. Pursue scientific opportunities and grand challenges in high energy density plasma science to explore the feasibility of the inertial confinement approach as a fusion energy source, to better understand our universe, and to enhance national security and economic competitiveness.
20. Increase the fundamental understanding of basic plasma science, including both burning plasma and low temperature plasma science and engineering, to enhance economic competitiveness, and to create opportunities for a broader range of science-based applications.

HEP

21. Understand the properties and interactions of the elementary particles and fundamental forces of nature from studies at the highest energies available with particle accelerators.
22. Understand the fundamental symmetries that govern the interactions of elementary particles from studies of rare or very subtle processes, requiring high intensity particle beams, and/or high precision, ultra-sensitive detectors.
23. Obtain new insight and new information about elementary particles and fundamental forces from observations of naturally occurring processes -- those which do not require particle accelerators.
24. Conceive, plan, design, construct, and operate forefront scientific user facilities to advance the mission of the program and deliver significant results.
25. Steward a national accelerator science program with a strategy that is drawn from an inclusive perspective of the field; involves stakeholders in industry, medicine and other branches of science; aims to maintain core competencies and a trained workforce in this field; and meets the science needs of the SC community.
26. Foster integration of the research with the work of other organizations in DOE, in other agencies and in other nations to optimize the use of the resources available in achieving scientific goals.

NP

27. To search for yet undiscovered forms of nuclear matter and to understand the existence and properties of nuclear matter under extreme conditions, including that which existed at the beginning of the universe.
28. Understand how protons and neutrons combine to form atomic nuclei and how these nuclei have emerged during the 13.7 billion years since the origin of the cosmos.
29. Understand the fundamental properties of the neutron and the neutrino, and how these illuminate the matter-antimatter asymmetry of the universe and physics beyond the Standard Model.
30. Conceive, plan, design, construct, and operate forefront national scientific user facilities for scientific and technical advances which advance the understanding of nuclear matter and result in new competencies and innovation. To develop new detector and accelerator technologies that will advance NP mission priorities.
31. Provide stewardship of isotope production and technologies to advance important applications, research and tools for the nation.
32. Foster integration of the research with the work of other organizations in DOE, such as in next generation nuclear reactors and nuclear forensics, and in other agencies and nations to optimize the use of the resources available in achieving scientific goals.

WDTS

33. Increase the pipeline of talent pursuing research important to the SC.
34. Leveraging the unique opportunities at DOE national laboratories to provide mentored research experiences to undergraduate students and faculty).
35. Increase participation of under-represented students and faculty in STEM programs.
36. Improve methods of evaluation of effectiveness of programs and impact on STEM workforce.

Energy Security (ES)

1. Supply - Solar
2. Supply - Nuclear
3. Supply - Hydro
4. Supply - Wind
5. Supply - Geothermal
6. Supply - Natural gas
7. Supply - Coal
8. Supply - Bioenergy/Biofuels
9. Supply - Carbon capture and storage
10. Distribution - Electric Grid
11. Distribution - Hydrogen and Gas Infrastructure
12. Distribution - Liquid Fuels
13. Use - Industrial Technologies (including efficiency and conservation)
14. Use - Advanced Building Systems (including efficiency and conservation)

15. Use - Vehicle Technologies (including efficiency and conservation)
16. Energy Systems Assessment/Optimization

Environmental Management (EM)

1. Facility D&D
2. Groundwater and Soil Remediation
3. Waste Processing

National Security (NNSA)

1. Stockpile Stewardship and Nuclear Weapons Infrastructure
2. Nonproliferation
3. Nuclear Propulsion

Homeland Security (HS)

1. Border Security
2. Cargo Security
3. Chemical/Biological Defense
4. Cyber Security
5. Transportation Security
6. Counter-IED
7. Incident Management
8. Information Sharing
9. Infrastructure Protection
10. Interoperability
11. Maritime Security
12. Human Factors

Appendix 3 Integrated Facilities and Infrastructure Budget Schedule

Core Capabilities		Mission Ready, Assumes TYSP Implemented				Key Buildings	Facility and Infrastructure Capability Gap	Action Plan	
		N	M	P	C			Laboratory	DOE
Chemical and Molecular Sciences	Now	X				EMSL, PSL, RTL	The EMSL large instrumentation and chemical synthesis laboratory space is fully subscribed, chemical and molecular sciences capabilities less aligned to EMSL User Program need to be relocated outside EMSL to address overcrowding. PSL building design cannot support chemical and molecular sciences' need for hood-intensive, chemical synthesis laboratories or vibration and EMF-isolated imaging suites. Dated laboratory layouts and fixed casework limit research productivity and make housing analytical equipment a challenge. Even under these conditions, PSL is fully subscribed hampering renewal. Approximately 18,000 nsf of vacated contiguous space is needed to accommodate the renewal construction work. A completed FY 2010 laboratory optimization study identified several stop-gap actions to help accommodate ongoing work.	Near-term, individual optimization projects are underway to increase utilization of existing laboratories. Long-term, PSL will be upgraded for energy conversion activities. Projects: Various optimization; PSL renovation-multiyear.	Construct 100,000 gsf to provide chemical synthesis and imaging laboratories adjacent to materials and process development efforts. This envisioned facility is configured to bring science and applied core capabilities together to create clean energy sources. Project: CSIL line item.
Climate Change Science	Now				X	AML, JGCRI, ARM,	Additional mid-scale computing resources are needed to support regional and global climate and Earth system modeling activities. Upgrading AML interior finishes and securing additional office space for atmospheric sciences and global change personnel in Richland would also be desirable.	Requirements for additional mid-scale computing resources are currently being evaluated and incorporated into PNNL computing strategy.	Design and implement a plan to build a National Atmospheric Laboratory Facility for studying cloud and aerosol processes, a programmatic facility need recognized by DOE's Atmospheric Systems Research program that PNNL is uniquely qualified to fill.
	In 5 Years			X					
	In 10 Years			X					
Biological Systems Science	Now				X	BSEL, BSF, EMSL, CSF, MSL, BIL	With the exception of off-campus MSL, all facilities are newly constructed or fully functional. By agreement with WSU, PNNL's BSEL footprint is limited. BIL acquisition relieves work with dispersible radioactive material by offloading 331 in near-term.	Project: 331 Building Filter Exhaust; Aquatic laboratory upgrades.	
	In 5 Years				X				
	In 10 Years			X					
Environmental Subsurface Science	Now				X	331, MSL, Sigma 5, RTL, EMSL	In general existing space meets functional needs, though staff and equipment could be better located to enhance collaboration.	Upgrades to 331Aquatics Laboratory and radiological labs provide modernized capabilities. Projects: 331 Aquatics Lab and Lab optimizations.	Construct 100,000 gsf to provide materials synthesis and scale-up demonstration laboratories adjacent to fundamental science efforts. This facility is envisioned to bring science and applied core capabilities together to create clean energy sources. Project: CSIL line item.
	In 5 Years				X				
	In 10 Years				X				

Core Capabilities		Mission Ready, Assumes TYSP Implemented				Key Buildings	Facility and Infrastructure Capability Gap	Action Plan	
		N	M	P	C			Laboratory	DOE
Advanced Computer Science, Visualization and Data	Now			X		CSF, SEF, ISB1 ISB2 EMSL	Classified and unclassified computer technology and computational staff count and equipment inventory continue to grow out pacing available space and facility/site infrastructure. Newly leased SEF space addresses office needs. EMSL and CSF infra-structure upgrades (FY11 and FY12 projects) partially addressed classified computing space and supporting infrastructure needs.	Campus computing consolidating and high performance computing SCIF will allow for full utilization of computational space. Projects: Campus computing consolidation; High Performance SCIF.	
	In 5 Years				X				
	In 10 Years				X				
Applied Nuclear Science and Technology	Now			X		318, 325, 331, PSF (3410, 3420, 3425, 3430, 3440)	The newly constructed PSF and the 300 Area 318 and 325 buildings are fully functional. Additional radiochemistry and sensor development laboratories are required to address anticipated rapid growth in signature science. Additionally a small part of this core capability is located in an off-campus leased office and instrumentation development laboratory facility. Efficiencies and collaborative opportunities can be gained by locating this core capability on the PNNL campus. Note: Though replacement of the 325 CAT II facility is outside of the 10-year planning period, the planning for replacement has commenced.	Various upgrades to 325 Building laboratory configurations and capabilities are needed to fully enable this core capability in the near term. Additional PSF office space will be provided through staff relocations. Longer term, it will be necessary to replace off-campus leased space driving the need for additional office space near PSF. Projects: Various 325 laboratory optimization projects and B-Cell replacement window; PSF Office building.	Complete 300,000 gsf new construction to replace 300A capabilities and meet planned 2026 exit. Projects: 300 Area Phase II Capability Replacement.
	In 5 Years			X					
	In 10 Years			X					
Applied Material Science and Engineering	Now				X	PSF (3410), RTL, APEL, PSL, EMSL	PSF and EMSL are fully functional and fully subscribed. The availability of space and building utility systems has limited the use of PSL and RTL. APEL is a Port of Benton incubator facility remote from the PNNL campus in which PNNL leases a limited amount (amount is limited by written agreement) of materials development and high ceiling process development laboratory and office space. Hood capacity in APEL is limited.	The additional optimization projects will relocate several PSL and RTL research organizations to improve adjacencies. Longer term, it will be necessary to replace off-campus leased APEL space. Projects: Various PSL, RTL, laboratory optimization projects.	Provide swing space to renovate on-campus facilities to replace off-campus leased APEL. Projects: CSIL line item.
	In 5 Years				X				
	In 10 Years				X				
Chemical Engineering	Now			X		BSEL, PSL, RPL, APEL	BSEL, the relatively new WSU joint-partner facility, is fully functional for its use. APEL is a Port of Benton incubator facility remote from the PNNL campus in which PNNL leases a limited amount of chemistry, high ceiling process development, and office space. APEL hood capacity is limited. Chemical engineering activities housed in PSL face the same challenges as others in adequate hood capacity, dated and inflexible laboratory configurations.	The additional optimization projects will relocate several PSL and RTL research organizations to improve adjacencies. Longer term, it will be necessary to replace off-campus leased APEL space. Projects: Various laboratory optimization projects.	Complete 100,000 gsf new construction to provide process engineering laboratories and high bay space adjacent to fundamental science effort. This facility is envisioned configured to bring science and applied core capabilities together to create clean energy sources. Project: CSIL line item.
	In 5 Years			X					
	In 10 Years				X				

Core Capabilities		Mission Ready, Assumes TYSP Implemented N	M	P	C	Key Buildings	Facility and Infrastructure Capability Gap	Action Plan: Laboratory	Action Plan: DOE
Systems Engineering and Integration	Now				X	PSF (3420, 3440), Math, SEF, 2400 Stevens	The newly constructed PSF provides replacement laboratories supporting radiation portal monitoring activities. The Math Building which houses systems engineering and integration computational and visualization laboratories may require building utility system upgrades in cooling, and humidity control. Multiple on-campus and off-campus leased facilities house required instrument development laboratories, and classified office and laboratory space. Efficiencies and collaborative opportunities can be gained by locating this core capability on the PNNL campus.	Math Building infrastructure was upgraded to address cooling and humidity control issues. Lease acquisitions are addressing the need for expanded classified and non-classified office, computational space, and classified instrument development space. Longer term, it will be necessary to replace off-campus leased space, 2400 Stevens. Projects: Power Engineering Research Laboratory (PERL).	
	In 5 Years				X				
	In 10 Years				X				
Large-Scale User Facilities/ Advanced Instrumentation	Now			X		EMSL, ARM	The EMSL unique large instrumentation and chemical synthesis laboratory space is fully functional and fully subscribed. Estimates are approximately 13,000 nsf of laboratory space is needed to address current overcrowding. Planned (beyond FY12 project) expansion in computational capacity will require increased electrical power and cooling.	Decisions involving CSIL options analysis will determine final location of the relocated less aligned programs in EMSL. Projects: CSIL and RTL modifications	Programmatic GPP provided specialty laboratory space in FY12 and will continue to provide specialty space as needs emerge. Continued growth in the EMSL program would drive the need for an EMSL North Laboratory and Office Pod. Project: EMSL North Pod Expansion.
	In 5 Years				X				
	In 10 Years				X				

325 Building	=	Radiochemical Processing Laboratory	JGCRI	=	Joint Global Change Research Institute
AML	=	Atmospheric Measurements Laboratory	LSL-II	=	Life Sciences Laboratory II
APEL	=	Applied Process Engineering Laboratory	M	=	marginal
ARM	=	Atmospheric Radiation Measurement Climate Research Facility	MSL	=	Marine Sciences Laboratory
BIL	=	Battelle Inhalation Laboratory	N	=	not
BSEL	=	Bioproducts, Sciences, and Engineering Laboratory	PERL	=	Power Engineering Research Laboratory
BSF	=	Biological Sciences Facility	nsf	=	net square feet
C	=	capable	P	=	partial
CSF	=	Computational Sciences Facility	PSF	=	Physical Sciences Facility
CSIL	=	Chemical Sciences and Imaging Laboratory	PSL	=	Physical Sciences Laboratory
DOE	=	U.S. Department of Energy	RPL	=	Radiochemical Processing Laboratory (325 Building)
EMF	=	electromagnetic field	RTL	=	Research Technology Laboratory
EMSL	=	Environmental Molecular Sciences Laboratory	TYSP	=	Ten-Year Site Plan
GPP	=	general plant project	WSU	=	Washington State University
gsf	=	gross square feet			

Appendix 4 Support Facilities and Infrastructure

Real Property Capability	Mission Ready Current N	M	P	C	Facility and Infrastructure Capability Gap	Action Plan Laboratory	DOE
Work Environment			X		Various on-site amenities are inadequate including conferencing and food center, and fitness center. A lack of storage facilities result in not-in-use materials and equipment stored in offices and laboratories.	PNNL "The Center" purposed within planning period	
User Accommodations			X		Various on-site amenities are inadequate, including conferencing and food center, and fitness center.	PNNL "The Center" purposed within planning period	
Site Services			X		Maintenance and fabrication facilities are in a poor condition and/or location. These facilities are over-subscribed.	Central Operations Building, Central Machine Shop	
Conference and Collaboration Space			X		Amount of collaboratory space is below industry standards. On-site conferencing space is less than required.	PNNL "The Center" purposed within planning period	
Utilities			X		A limited amount of compliance-driven upgrades to water system back flow preventors is required. An increase in the reliability of electrical distribution system, and a decrease in energy and water usage are required.	BMI-funded backflow preventor installation; EMSL Electrical Infrastructure Upgrade (City of Richland)	
Roads and Grounds			X		General end-of-life issues	Various road and grounds projects (BMI)	
Security Infrastructure			X		Security operations are transferring to PNNL from an outside provider. To meet future needs, a new security operation building or existing facility modification is envisioned to house equipment and operations.	Central Security Operations	

NOTE: Current plans address technical facilities and infrastructure ahead of the support facilities.

BMI = Battelle Memorial Institute
C = capable
DOE = U.S. Department of Energy
EMSL = Environmental Molecular Sciences Laboratory
M = marginal
N = not
P = partial
PNNL = Pacific Northwest National Laboratory
PSF = Physical Sciences Facility

Appendix 5 PNNL Lease Actions and Expiration Portfolio

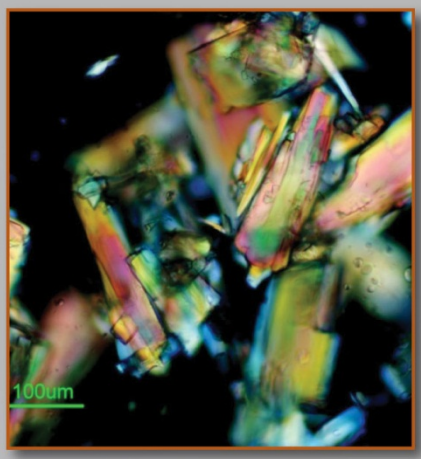
PNNL Near-Term Lease Actions and Expiration Portfolio for Leases with Greater than 10,000 ft^2 of Space

Near-Term Lease Actions	FY 2012	FY 2013
Contractor Leased	1,081,000	1,061,000
Planned Exit (Sig3, partial 2400 Stevens)	(20,000)	(16,250)
Additions (BMI)	--	391,000
Total	**1,061,000**	**1,435,750**

Leased Portfolio Expirations	FY 2012	FY 2013	FY 2014	FY 2015	FY 2016	FY 2017
Sigma 3	20,000					
2400 Stevens	102,000					
APEL	49,000					
Port of Pasco (Hanger)	10,000					
Sigma 1	20,000					
BIL (ILA)	16,000					
LSL (ILA)	14,000					
Seattle (ILA)	30,000					
Sigma 2		20,000				
JGCRI (Maryland)			18000			
LSB			84000			
Sigma 4				21000		
Salk					10000	
Sigma 5					48000	
SEF						48000
ISB1						50000
ISB2						60000
CIC (Library)						30000
Other (<10K)	30,000	3000	6000	23000		
Total (sq ft)	**291,000**	**23,000**	**108,000**	**44,000**	**58,000**	**188,000**

Note: Values are in ft^2

ON THE COVER:



Using expertise in material nuclear forensics, PNNL scientists and engineers are developing cutting-edge signature discovery tools related to the nuclear fuel cycle. This image of thorium nitrate and uranyl sulfate crystals was obtained from a Nikon 400 POL polarized light microscope (PLM) with cross-polars. The PLM provides unique insight into materials and enables rapid screening of unknowns. The cross-polars image of uranyl sulfate shows large 0.5-millimeter crystals exhibiting a wealth of interference colors. Contrasts in the images are due to thickness variations across the crystal, much like the interference colors from an oil slick on water. This work was jointly funded by NA-20 and National Technical Nuclear Forensics Center (NTNFC), and supports the Laboratory's major initiative in Signature Discovery and Exploitation for Threat Detection and Reduction. PNNL scientists Leah Arrigo and Crystal Rutherford contributed to the project, which is managed by Jon Schwantes. *This image was provided by PNNL scientist Edgar Buck.*

A metal-organic framework (MOF) composed of zinc nitrate and 2,5-dihydroxy terephthalic acid was imaged at 10,000-times magnification as part of a study to understand how nano-porous frameworks can be created and modified to improve gas capture properties. The MOF is part of a new series of materials developed by PNNL that have tiny "cages" that can be used to trap carbon dioxide. The crystals in the cages have a diameter of about 25 nanometers. The cages themselves consist of metal ions linked together with organic ligands forming a porous network that traps gas molecules. The unique molecules have two to three times the capacity for carbon dioxide uptake as conventional solvents and appear to have an extremely high preference for carbon dioxide over other gasses. This research was funded by BES, and supports the Laboratory's major initiative in Coupling Earth and Energy Systems for Sustainability. This image (in false color) was captured using a focused ion beam scanning electron microscope at EMSL, a DOE national scientific user facility. *Image provided by EMSL's Bruce Arey and PNNL's Carlos A. Fernandez and Praveen Thallapally.*

Microbe-mineral and -metal interactions represent a major intersection between the biosphere and geosphere but require high-resolution imaging and analytical tools for investigating microscale associations. Electron microscopy has been used extensively at PNNL for geo-microbial investigations such as the controlled exposure of model organism *Shewanella* to environmentally relevant metals and radionuclides to understand how microbes carry out complex biogeochemical processes. At EMSL, scientists are using the state-of-the-art instrumentation and expertise in electron microscopy imaging and analyses for research of the effects of the interactions of microbes with the soil environment. Shown here is a scanning electron micrograph of *Shewanella putrefaciens* CN-32 cells in certain conditions that induce cells flocculation. CN-32 is a metal-reducing bacteria important for stabilization of metals in the environment. This work was funded by BER, and supports the Laboratory's major initiative in Accelerating Innovation and Discovery and Transforming the Conduct of Science in the Environmental Molecular Sciences Laboratory (EMSL). *This research was carried out in PNNL's Microbiology group led by Jim Fredrickson, the image was provided by EMSL scientist Alice Dohnalkova.*

2013 Laboratory Plan

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