FWP Title: II: Correlated Materials – Synthesis and Physical Properties (Fisher/Beasley/Geballe/Kapitulnik/Kivelson/Moler)
FWP Number: #2009-SLAC-10028

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0202010 (new FY10: KC0201010)

Program Abstract:
This FWP is part of the newly formed Stanford Institute for Materials and Energy Sciences (SIMES), a joint venture between the SLAC National Accelerator Laboratory and Stanford University. Within our specific FWP, our efforts aim to address the grand challenge of "emergence" as well as a number of "Basic Research Needs" areas for energy applications in the realm of quantum materials. In broad terms, we seek to understand how complex interactions in strongly correlated electron systems lead to emergent quantum behavior, including unconventional superconductivity, charge and spin ordered states, and non-Fermi liquid behavior. We combine a range of techniques to address these questions, including crystal growth and characterization of novel materials (Fisher & Geballe), local electronic (Kapitulnik) and magnetic (Moler) measurements, and theory (Kivelson). Within the realm of superconductivity, we work with a variety of systems and families of compounds, ranging from the newly discovered iron arsenides, through cuprates, ruthenates, and materials based on valence skipping elements. We also work with a range of materials exhibiting broken symmetry states as a consequence of electron correlation (from charge ordered states in complex oxides to the weak-coupled analogs of simpler CDW materials), seeking to find unifying ideas. More recently, we have also worked on topological insulators, establishing synthesis techniques to obtain crystals with the lowest possible bulk carrier density, and developing probes that reveal the associated exotic properties. In all cases, our focus is on understanding the fundamental factors determining the often complex electronic properties of these materials from both from an experimental and theoretical perspective.

Program Impact:
Scientific results that address BES Grand Challenges:
Quantum materials have the potential to profoundly impact the next generation of electronic materials relevant to addressing our nation's energy needs. From new quantum states that enable computing with vastly lower power consumption, to new superconductors that better suit power transmission requirements, quantum materials hold the promise of advanced applications as well as providing some of the deepest intellectual questions. But to realize this potential there are significant challenges that must be met. Our research addresses the fundamental aspects governing the emergent quantum behavior in strongly correlated materials, with the long term goal of providing a foundation for technological applications of advanced electronic materials. This research is both highly interactive and highly interdisciplinary, finding a natural home in the newly formed Stanford Institute for Materials and Energy Sciences at SLAC National Accelerator Laboratory.
New materials for BES:
The search for and discovery of novel materials has long been acknowledged to play a vital role in the field of condensed matter and materials physics. The materials synthesis component of this FWP enables a wide range of experiments both within SIMES and also at other institutions via extensive collaboration.

FY 2009 Authorized Budget (New BA): $1,510,000

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
I. R. Fisher (PI-10%), M. R. Beasley (PI-10%), T. H. Geballe (PI-10%), A. Kapitulnik (PI-10%), K. Moler, (PI-10%), S.A. Kivelson (PI-10%), F. Kidwingira (PD-50%), A. Tsukada (PD-75%), Z. Alpichshev (GS-50%), J. Analytis (RA-50%), E. Berg (GS-50%), J. H. Chu (GS-50%), F. Corridor (GS-25%), A. Erickson (GS-30%), C. Hicks (GS-40%), H. Karapetyan (GS-50%), J. Kim (GS-15%), T. Lippman (GS-60%), L. Liu (GS-10%), L. Luan (GS-50%), K. Luna (GS-20%), K. Munakata (GS-30%), P. Oreto (GS-13%), E. Schemm (GS-50%), L. Zhang (GS-30%), C. Kucharczyk (S-50%)

Interactions:
A. Carrington (Bristol), J. R. Cooper (Cambridge University, UK), T. Devereaux (Stanford), H. D. Drew (Maryland), L. DiGiorgi (ETH Zürich, Switzerland), S. Dugdale (Bristol University, UK), C. Gough (Birmingham, UK), R. Hackl (Walther Meissner Institut, Germany), S. Hayden (Bristol), N. Hussey (Bristol University, UK), Z. Islam (APS, ANL), M. Johannes (NRL), A. Kaminski (Ames Lab), Y.J. Kim (Toronto), M. B. Maple (UCSD), I. Mazin (NRL), R. McDonald (NHMFL), J. Mesot (PSI, Switzerland), D. Mihailovic (Jozef Stefan Institute, Slovenia), J. Orenstein (Berkeley), J. Schmalian (Ames Lab), Z. X. Shen (Stanford), M. Toney (SSRL), M. Wolf (Freie Universität Berlin).

FWP Title: I: Electronic and Magnetic Structure of Quantum Materials (Devereaux)
FWP Number: #2009-SLAC-10027

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0202010

Program Abstract:

The first FWP focuses on the physics of correlated materials, with a strong emphasis on coupled theoretical and experimental activities, to probe and understand electronic and magnetic structures of complex materials. We study the fundamental principles governing the emergence of novel phases of quantum matter in correlated materials that derive from the strongly intertwined charge, spin, orbital, & lattice degrees of freedom. Our efforts aim to address the grand challenge of "emergence" as well as a number of Basic Research Needs areas for energy applications. The complex materials targeted for this research have strong ties to superconductivity and related phenomena, such as Solid State Lighting, for example. The insights, methodology, and experimental/theoretical tools developed also contribute to a general theme in modern research: transformation from science of observation to science of control.

Both experimental & theoretical advancements of x-ray spectroscopy, scattering, and imaging techniques offer unprecedented insights into electronic/magnetic structures in materials, & span areas from fundamental science to applied materials & devices. Our intellectual emphasis is to study novel charge, magnetic, orbital & superconducting order in a number of novel materials using tools and methods based on photon experiments & simulations.

Program Impact:

A collaborative approach utilizing many distinct areas of expertise is necessary to address dynamics in materials relating to energy science. Our FWP works collaboratively as a unit, resulting in 18 high profile papers in our focused research areas (Science, Phys. Rev. Lett., Nature, App. Phys. Lett, Nano Lett., Europhys. Lett, Optics Lett., PNAS) out of 37 papers during the past review period, plus two articles published in PRB selected as *Viewpoints in Physics*. We work collectively (18 joint-authored pubs) within our FWP (5) and all the other current and proposed FWPs of SIMES 13), leveraging activities in sample growth and fabrication, photon-science based expertise, and theoretical simulation and modeling, for example. We collaborate closely with the Advanced Light Source (11 joint publications), and functions as part of many international collaborations with diverse research areas.

We take advantage of two important Department of Energy (DOE) photon science user facilities at SLAC (SSRL and LCLS), related in-house experimental tools, as well as cutting edge theoretical capabilities both locally at SLAC and NERSC grid computing. We also leverage efforts with other DOE user facilities, such as the Advanced Light Source at Berkeley. The advanced X-ray capability is essential to address all 5 grand challenge problems because of its ability to reveal atomic and electronic structures on ultrasmall and ultrafast length and time scales.

FY 2009 Authorized Budget (New BA): $2,207,500

Program Personnel Supported in FY2009: T. P. Devereaux (PI-90%), Z.-X. Shen (PI- 10%), J. Stohr (PI-5%), R.Moore (Staff Scientist-10%), Andreas Scherz (Staff Scientist -75%), Y. Chen (Assoc Staff Scientist-100%), W.S. Lee (Assoc Staff Scientist -95%), P. Kirchmann (PD-45%), M. Hashimoto (RA-75%), B. Moritz (RA-95%), S. Sarkar (RA 25%), C.C. Chen (GS-45%), G. Chobot-Conture (GS-50%), C.Jia (GS-65%), R. He (GS-60%), H. Ishiwata (GS-50%), S. Johnston (GS-10%), Y. Li (GS-50%), Z. Liu (GS-50%), E. Motoyama (GS-50%), B. Nowadnick (GS-60%), Ramon Rick (GS-10%), D. Riley (GS-10%), F. Schmitt (GS-50%), I. Vishik (GS-50%), M. Yi (GS-50%), D. Zhu (GS-20%), L. Patthey (Visitor-20%), J. Van den Brink (Visiting Phys-40%)

Interactions: J. van den Brink (Dresden); R. R. P. Singh, R. T. Scalettar (UC-Davis); R. Hackl (WMI); D. J. Scalapino (UCSB); C. Kim (Yonsei); E. Rotenberg, Z. Hussain (LBNL); P. J. Hirschfeld (UFlorida); H. Eisaki, A. Fujimori, S. Uchida, N. Nagaosa (Tokyo); I. Mazin (NRL); D. J. Singh (ORNL); Y. Ando (Osaka); A. Balatsky (LANL); T. Xiang (Beijing); K. Shen (Cornell); N. Mannella (UTenn.); W. Wurth, A. Foehlisch (FLASH).

Related Project URL: http://simes.slac.stanford.edu/; http://stanford.edu/group/photontheory/; http://arpes.stanford.edu/; http://www-ssrl.slac.stanford.edu/stohrgroup/

FWP Title: IV: Interfaces and Catalysis for Energy Conversion and Storage (Nilsson/Mao)

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0202010

FWP Number: #2009-SLAC-10030

Program Abstract:

This program addresses chemical transformations involving interfaces where catalysis occurs or the change of materials under high pressure. Many of the essential processes in energy conversion, energy storage and reduced energy impacts on the environment involve chemical transformations at interfaces between solids and electrolyte solutions or gases. Our effort is related to the DOE Grand Challenge of understanding the "nano-scale communication" and "control of electrons" in interfacial problems and "matter in extreme conditions" regarding systems under high pressures. The program consists currently of two subtasks with focus on the usage of x-rays to characterize materials connected to interfacial processes in fuel cell catalysis and for hydrogen storage under high pressures.

Program Impact:

This program has the potential to have a large impact on the future Hydrogen Initiative. Fuel cells are currently considered as one of the most promising power generation technologies for a sustainable energy infrastructure and it is essential to solve the hydrogen storage problem. In order to make a scientific breakthrough it is essential to create a program that allows for strong interactions between various scientists but also with the current light sources.

FY 2009 Authorized Budget (New BA): $850,000

Program Personnel Supported in FY2009:

A. Nilsson (PI-10%), W. Mao (PI-60%), Strasser (PI-10%) (UH), M. Toney (Staff Scientist-10%), M. Baldini (PD-100%), L. Å. Näslund (PD-10%), D. Friebel (RA-60%), R. Yang (RA-100%), T. Anniyev (GS-50%), P. Mani (GS-100%) (UH), D. Miller (GS-50%), S. Wang (GS-50%), PS. Koh (S-100%) (UH).

Interactions:

There is a strong interaction between Nilsson, Toney and Strasser in fuel cell catalysis efforts. It involves catalysts preparation (Strasser), x-ray and electron spectroscopy (Nilsson) and x-ray scattering (Toney) measurements. Nilsson has a long term collaboration with Lars Pettersson in Stockholm regarding spectroscopy calculations.
University of Houston has a very active collaborative effort with Oak Ridge National Laboratory on STEM analysis of dealloyed high activity Pt-Cu nanoparticles. UH also has very close efforts together with the Technical University Berlin, Berlin, Germany. Furthermore collaborative work was performed together with Dr Jeff Greeley, Argonne National Laboratory on theoretical calculations of the fuel cell processes on strained catalysts..
Mao and Nilsson collaborate with Devereaux in FWP I regarding theory for x-ray and Raman spectroscopies. Mao is starting an interaction with Melosh and Shen on the Diamondoid SISGR looking at these novel carbon-based nanomaterials at extreme conditions. Mao is developing high pressure x-ray spectroscopy and high resolution imaging capabilities at SSRL in collaboration with Nilsson, U. Bergmann, D. Nordlund, and P. Pianetta.
Mao has established collaborations with researchers and at the Geophysical Laboratory including R. Hemley, H.K. Mao, and V. Struzhkin. We are beginning collaborations with theoreticians including P. Cummings (Vanderbilt), R. Ahuja (Uppsala University), and Wei Luo (Uppsala University), and M. Kroon (Technical University of Delft) as well as other experimentalists including P. Lazor (Uppsala University), and J. Chen (Florida International University).

FWP Title: VI: Time-Resolved Soft X-ray Materials Science at the LCLS & ALS (Devereaux/Shen)
FWP Number: #2009-SLAC-10017

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0202010

Program Abstract:
The purpose of this research is to develop a world class program on the dynamics of complex materials using the soft x-ray beamline available at the Linac Coherent Light Source (LCLS) at SLAC to address the grand challenge problems of "emergence", and to probe model systems for deep insights on materials for energy conversion, transport and efficiency. We propose performing time-resolved, optical-pump and x-ray probe, momentum-resolved x-ray scattering on strongly correlated materials utilizing the ultra-short soft x-ray pulse produced by the SXR beamline of LCLS. Theoretical calculations will be performed in parallel to gain further insight into the experimental data and to establish a formalism for describing non-equilibrium physics of strongly correlated materials. The program consists of a local core team made of researchers from SLAC and Lawrence Berkeley National Laboratory (LBNL), enhanced by a strong web of collaborations with scientists from other institutions.

Program Impact:
The technological and scientific coverage of this program is extremely broad, outside the range of a single PI. Experimentally, the program intimately connects technology developed for ultrafast, time-domain science with that for momentum- and energy-domain x-ray spectroscopy. Thus a joint effort between experimental groups at SIMES at SLAC and the Advanced Light Source at LBNL with the respective expertise is necessary for the future success of the proposed activity. To understand the data generated from the experimental component of the SISGR activity, novel theoretical tools must be developed whose aim is to uncover the nature of the many-body state in- and out-of-equilibrium. The SISGR program combines expertise in both experimental and theoretical and computational areas to ensure that the program has a maximal chance of successfully achieving its goals.

FY 2009 Authorized Budget (New BA): $400,000

Program Personnel Supported in FY2009:
T.P. Devereaux (PI-5%), Z.X. Shen (PI-5%), B. Moritz (RA-5%), W.S. Lee (RA-5%)

Interactions:
Experimentally, our team and the ALS team have worked very closely on the construction of a chamber suitable for performing resonant soft x-ray scattering during our LCLS beamtime scheduled for Summer 2010. Meanwhile, optical construction and calibration for the spectrograph is currently in progress. Frequent informal meetings among the different groups represented in the proposal are held to update progress on different aspects of the activity. We have also formed collaborations with other groups outside our SISGR proposal to enhance our experience in cut-edge x-ray scattering and ultrafast experiments.

Ultrafast Experiment: We collaborate with the group of Robert Schoenlein at ALS to perform ultrafast optical pump-probe experiments on stripe-phase nickelates. This provides useful experimental parameters and scientific guidance for our LCLS experiment in Summer 2010.

Resonant Inelastic Soft X-ray Scattering Experiment (RIXS): We have formed a collaboration with the RIXS group lead by Dr. Luc Patthey and Thorsten Schmitt at the Swiss Light Source, Switzerland. Through this collaboration, we have performed RIXS experiments on stripe-phase nickelates in December 2009. More experiments will be performed beginning in February 2010.

The theory and computation team has begun collaborating with a group external to the core team of our SISGR proposal to enhance our understanding of non-equilibrium phenomena in strongly correlated systems.

Photoemission response of correlated systems out-of-equilibrium: We have started our work on ultrafast, nonequilibrium phenomena in strongly correlated systems in collaboration with J. Freericks, Georgetown Univ. These investigations had been facilitated in 2009 by an Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award at the National Energy Research Scientific Computing Center (NERSC) and are currently facilitated by a DOE Production grant at NERSC.

Related Project URL: http://www.stanford.edu/group/photontheory/cgi-bin/wiki1/

FWP Title: VIII: Modern Angle-Resolved Photoemission Spectroscopy Beamline for the Study of Complex Phenomena in Solids (Lu/Shen)

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0202010

FWP Number: #2009-SLAC-10016

Program Abstract:
Angle-resolved photoemission spectroscopy has emerged as a leading experimental probe for studying the "emerging phenomena" in quantum materials, a subject of increasing importance. This technique, as well as the advanced version that resolves the spin quantum number, will continue to be at the forefront of materials research in addressing the important grand challenge problems. To realize the full potential of this technique and to capitalize the new capabilities presented by the SPEAR3 upgrade, we propose to build a new undulator beamline with variable polarization control, covering the photon energy range of 10-150 eV. It will completely modernize and greatly expand the capabilities of the ten-year old NIM branch-line on the same straight section with more polarization control, extended photon energy range, and significant improvement in flux and spot size. Along with the NIM branch-line and the experimental stations developed separately, the proposed facility features several capabilities that are either unique or rare among the existing synchrotron facilities in US, enabling new classes of science that otherwise cannot be done. Once completed this beamline/end-stations combination will become a leading photoemission facility in the world. We envision that this new beam line will have most of its beam time for general users.

Program Impact:
The objective of the program is to build a state-of-the-art photoemission beamline at SSRL and to develop a forefront scientific program at this facility. The proposed research program addresses a number of critical energy needs outlined in the BES Basics Research Needs Reports – superconductivity, solar energy utilization, solid state lighting and catalysis. In forming a strong scientific team to cover the broad scope of the research program we bring together a group of scientists from all over the world with diverse yet overlapping interest and background. They all share common interest in the proposed facility and would work together to deliver a beamline that will enrich a wide range of scientific areas. We will make every effort to stimulate collaborations among the scientific teams so that the scientific program will be more than just the sum of a few individual programs. With the expertise of PIs and participating scientists in all of the important research directions proposed in this document, we expect to make strong scientific impact in a number of different topics and push the frontier of complex phenomenon in solids.

FY 2009 Authorized Budget (New BA): $3,600,000

Program Personnel Supported in FY2009:
T. Rabedeau (Staff Scientist – 10%)

Interactions:
At this initial stage of the new beamline development, the interactions are mostly between the Beamline Construction Management Team (D. Lu, R.G. Moore, P. Pianetta, Z.-X. Shen, Z. Hussain) and the SSRL Beamline Development (BLD) Group.

Related Project URL:

FWP Title: III: Spin Physics (Zhang) **SLAC National Accelerator Laboratory - SIMES**
(Acremann /Goldhaber-Gordon/Manoharan/Orenstein/Stohr) **B&R Code: KC0202020 and KC0202030**

FWP Number: #2009-SLAC-10029

Program Abstract:
The spin physics program consists of three closely related subtasks. The first subtask investigates spin transport in semiconductors and metals. An important objective of semiconductor spintronics is to generate the electron spin polarization, and to preserve it for sufficient time for possible information processing. On one hand, spin-orbit coupling could enable electric or optical generation of the spin polarization; however, on the other hand, it could also lead to the rapid decay of the spin life time. The collaboration between Orenstein and Zhang groups showed both theoretically and experimentally that the Rashba and the Dresselhaus spin-orbit couplings could compensate each other, so that a persistent-spin-helix (PSH) with enhanced life time is obtained. Under an applied electric field, the induced spin currents lead to a phase shift of the PSH, which can be probed by our optical grating experiment. The second subtask investigates nano-magnetism. Over the last decade, spin physics has transformed information technology through the widespread use of the giant-magnetoresistance (GMR) effect. In GMR, the dependence of the flow of spins on the magnetization direction in a sensor is used to read information. The opposite "spin torque" (ST) effect is based on the use of a spin current to write information through switching a magnetic bit. The subtask of Stohr and Acreman is designed to understand and probe the processes associated with the manipulation of the magnetization of a magnetic nanostructure by spin currents, in both space and time, through the Scanning Transmission X-ray Microscopy (STXM). The third subtask of Goldhaber-Gordon and Manoharan will directly measure and manipulate low-dimensional spin, isospin and electron correlations using tunneling measurements (STM, a new tool termed "Virtual STM", and quantum transport) and via the precise control of nanoscale geometry through nanofabrication and nanoassembly. In nanoassembled materials Manoharan's group has been mapping the effects of quantum mechanical phase in various forms, guided by the physics of real-space and k-space exact degeneracies in band structure. Goldhaber-Gordon's work involves manipulation of orbital moments through the creation of zero-field and zero-energy Landau levels in HgTe and graphene, respectively.

Program Impact:
Theoretical prediction of a new class of topological insulators Bi2Te3, Bi2Se3 and Sb2Te3 by Zhang's group launched an intense worldwide effort in this field. Several FWPs within SIMES worked closely on the experimental observation of the topological surface states. SIMES is now a recognized world leader in this field, and the work is highlighted in a feature cover article in Physics Today. The experimental discovery of the "Persistent Spin Helix" (PSH), a phenomenon predicted by Zhang, Orenstein and Bernevig, generated great interest. The Nature paper was highlighted in Physics Today and Online Journal Club. Manoharan's work on quantum holographic captured the public imagination, and was featured on the cover of the **NNI and Presidential FY2010 budget request.**

FY 2009 Authorized Budget (New BA): $ 1,004,500

Program Personnel Supported in FY2009:
S.C. Zhang (PI-40%), D. Goldhaber-Gordon (PI-10%), H. Manoharan (PI-10%), J. Orenstein (PI-10%), J. Stohr (PI-5%), Y. Acremann (Staff Scientist-25%), M. Baenninger (PD-50%), K. Gomes (PD-35%), M. Koenig (PD-100%), B. Bräeuer (RA-50%), X. Qi (RA-100%), D. Bernstein (GS-50%), K. Fang (GS-20%), A. Garcia (GS-50%), M. Hossain (GS-45%), R. Li (GS-50%), L. Mattos (GS-25%), C. R. Moon (GS-15%), M. Pelliccione (GS-50%), J. Randel (GS-25%), A. Sciambi (GS-50%), Y. Shi (GS-10%), X. Yu (GS-40%), Q. Liu (Visitor 100%), J. Wang (Visitor 100%)

Interactions: A. Bernevig (Princeton), Mike Lilly (CINT, Sandia), D. Awschalom (UCSB), A. V. Balatsky (LANL), K. Sengupta (SINP), W. de Heer (GaTech), L. Molenkamp (Wuerzburg), A. Gossard (UCSB) J. Reno (Sandia), M. Lilly (Sandia), L. P. Pfeiffer (Princeton), K. W. West (Princeton), B. Spivak (Washington), S. Kivelson (Stanford)

FWP Title: 0: Stanford Institute for Materials and Energy Sciences (SIMES) Administration

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0202020

FWP Number: #2009-SLAC-10048

Program Abstract:
This FWP supports the ongoing management and administrative costs for the SIMES Material Sciences program under the direction of PI, Zhi-Xun Shen. The administrative group supplies budgeting, financial planning, purchasing, reporting, payroll and travel support, as well as supporting safety and compliance functions.

Program Impact:

Provided critical mission support so that the researchers can work most efficiently to conduct forefront research. SIMES had a very successful FY2009 year in producing many high impact results, and the mission support unit played a critical enabling role.

FY 2009 Authorized Budget (New BA): $487,000

Program Personnel Supported in FY2009:
N. Matlin (Staff- 85%), E. Lwin (Staff- 49%), C. Meng (Staff- 25%), C. Peng (Staff- 100%), Y. Wackerman (Staff- 10%),

Interactions: NA

This activity provided the critical mission support needs of the program. As SLAC has not fully made the transition from a single program laboratory to a multi-program laboratory, the mission support activity in FY09 is still structured as a direct charge.

FWP Title: V: Carbon-based and Biomimetic Hybrid Materials (Heilshorn)
(Doniach/ Melosh/ Brongersma / McGehee/ Spakowitz)
FWP Number: #2009-SLAC-10031

SLAC National Accelerator Laboratory - SIMES
B&R Code: KC0203010

Program Abstract:
Self-assembly has become a powerful method to create highly-ordered structures with spatial and temporal patterning on two-dimensional substrates. However, there remains a vast divide between our current technological capabilities and the power demonstrated by biological systems to assemble both organic and inorganic species into intricate three-dimensional structures. The ultimate goal of this program is to identify the necessary combination of assembly mechanisms and building-block properties for deterministic formation of complex three-dimensional organic/inorganic constructs. By appropriate selection of architecture, materials, and morphology; these materials will lead to fundamentally new designs for bio-inorganic devices for energy storage, catalysis, solar cells, and fuel cells. Previous work in this area has focused on developing a fundamental understanding of the self-assembly of conjugated polymers and how this assembly dictates electronic properties for solar cell applications. Our recent collaborative effort has focused on the remarkable self-assembling protein, clathrin. Clathrin is composed of three-armed "triskelion" monomers, with three-fold symmetry, semi-flexible arms, and specific binding sites for adaptor peptide sequences. Clathrin is a highly unusual self-assembling material, as it occurs naturally in 2D sheets, 3D cubes, tetragons, and geodesic spheres. Because of the rich diversity of structure and dimensionality, clathrin is an ideal model for understanding how natural systems controllably transform from inherently two-dimensional materials into the third dimension. Our program combines experimental and theoretical approaches to demonstrate clathrin as a controllable 2D and 3D assembly system, identify the key self-assembly characteristics that make it successful, and finally template inorganic species to the clathrin networks.

Program Impact:
Successful development of a biotemplate for nanoscale architectures requires expertise in a diverse range of experimental and theoretical disciplines including polymer physics, inorganic chemistry, and protein science. Previous studies by others on clathrin self-assembly were narrowly focused on biological behaviors that are outside the conditions for biomineralization to occur. Therefore, DOE-BES funding allows us to greatly expand the existing knowledge of self-assembly to conditions that are more amenable to a flexible, nano-scale biotemplate system for applications in energy storage and production. This multidisciplinary research endeavor demands use of multiple physical and biological characterization techniques coupled with theoretical modeling to aid in the interpretation of results. This project would be impossible to successfully complete on a single PI level and without the unique characterization resources available through the DOE laboratories.

FY 2009 Authorized Budget (New BA): $550,000

Program Personnel Supported in FY2009 to Nearest +/- 10% FTE:
S.C. Heilshorn (PI- 10%), Brongersma (PI-10%), S. Doniach (PI-10%), McGehee (PI-10%), Melosh (PI-20%), A.J. Spakowitz (PI-20%), R. Gysel (PD-45%), Z. Beiley (GS-25%), A. Black-Schaffer (GS-25%), D. Boinagrov (GS-10%), N. Cordella (GS-40%), J. Fabbri (GS-50%), J. Lui (GS-50%), M. Rowell (GS-50), A. Schoen (GS-25%), B. Sudhanshu (GS-15%), M. Topinka (RA-10%), J. VanDersarl (GS-40%).

Interactions:
Michael Toney, SLAC, expertise in grazing incidence SAXS experiments
Gerald Fuller, Stanford University, expertise in interfacial rheometry for mechanical analysis of clathrin assemblies

Related Project URL: http://www.stanford.edu/group/heilshorn/Biotemplating/biotemplatehome.html

FWP Title: VII: Diamondoid Science and Applications (Melosh/ Devereaux/ Manoharan/ Shen/ Schreiner)

SLAC National Accelerator Laboratory - SIMES

B&R Code: KC0203010

FWP Number: #2009-SLAC-10018

Program Abstract:

Diamondoids are unique nanomaterials due to their sp^3 hybridization, atomic-level uniformity, flexible chemical functionalization, and systematic series of sizes, shapes and chiralities. This family of new carbon nanomaterials is an ideal platform for approaching the grand challenges of energy flow at the nanoscale and synthesis of atomically perfect new forms of matter with better precision than any other nanomaterials system. Diamondoids also offer more mechanical and chemical stability compared to other small molecule systems, and vastly superior size and shape control compared to inorganic nanoparticles. Electron transport and energy flow at the nanoscale is a delicate balance of interactions between species with quantized and band-like electronic structures, energy level alignment, and wavefunction overlap. This program systematically deconstructs these concepts by first understanding the properties of a series of isolated molecular units, then thin films, and finally bulk materials. Equally important, atomically-perfect organization of these functional units can be achieved for enhanced control of electron emission, tunneling, exchange, and rectification. Beyond these principle challenges, diamondoids provide a unique opportunity to broadly address the underlying theme of how quantum mechanical phenomena impact behavior at nano-lengthscales and femto-second timescales.

We have chosen to focus on following areas of research:

- Establish synthesis and assembly techniques for individual molecules, molecular monolayers, and thin films (Manoharan, Melosh, Schreiner)
- Understand how band gap and band alignment arise from diamondoid size, isomer, orientation, and chemical modification such as buckyball-diamondoid conjugate, related optical and fluorescence properties (Devereaux, Melosh, Shen)
- Diamondoids for high seeding density diamond film growth, properties and applications; mechanism of seeding and film growth mechanism at the interface; electron and photo-emission processes of diamondiods and related films.

Program Impact:

This program explores and develops diamondoids as a new class of functional nanomaterials based upon their unique electronic, mechanical, and structural properties. This includes all phases of investigation, including diamondoid isolation from petroleum, chemical functionalization, and molecular assembly, as well as electronic, optical and theoretical characterization. This naturally requires the broad expertise and collaboration between a number of investigators to successfully approach tackle these problems. This approach has yielded fruit, enabling synthesis of a number of new compounds, and exploration of their structural and electronic properties. In particular the ability of these materials to control the flow of electrons at the molecular level is an exciting direction for mastering energy flow at the nanoscale. The team meets biweekly to review current progress and new ideas often result from these meetings.

Diamondoids provide a systematic hierarchy of different molecular sizes and shapes with perfectly defined nanoscale atomic order which is an ideal system to study the role of quantum and structural effects at the nanoscale. This project will create a new materials platform that a number of BES investigators can take advantage of, providing unique materials for in-depth characterization using the LCLS, synchrotron and neutron scattering facilities.

FY 2009 Authorized Budget (New BA): $800,000

Program Personnel Supported in FY2009:

N. Melosh (PI-5%), T.P. Devereaux (PI-5%), H. Manoharan (PI-5%), Z.X. Shen (PI-5%), J. Dahl (Staff Scientist-10%), J. Randel (GS-5%), W. Clay (GS-5%), H. Ishiwata (GS-5%).

Interactions:

Zahid Hussien, LBL and Yi Cui, Stanford

Related Project URL: NA

FWP Title: "PULSE:The Stanford Photon Ultrafast Science and Engineering Center

Laboratory Name: SLAC National Accelerator Laboratory-PULSE

FWP Number: SCW0063

B&R Code: KC0202010

Program Abstract:

Subtask D.2.a: Experiments with variable bunch length

This program investigates the interactions of highly relativistic electron bunches with thin film metallic ferromagnets. It utilizes bunches of equal total energies but variable temporal durations to create electromagnetic field pulses with variable peak field values and frequency spectrums. The shortest bunches have unprecedented maximum electric and magnetic fields and closely resemble terahertz half cycle pulses. Such unique excitations are of great current interest in not only magnetism, but also many other areas of fundamental research and practical applications. Special emphasis here is placed on using these pulses to understand the dynamics of ultrafast magnetic switching in common ferromagnetic systems, such as those used for high density magnetic recording and spintronic applications.

Program Impact:

The study of ultrafast magnetization dynamics as discussed above requires access to SLAC's unique facilities to conduct the experiments and expertise in the understanding of magnetization dynamics at the nanoscale to interpret them. This distinctive combination enabled the program to reveal an electric field induced magnetic anisotropy in a thin film ferromagnet due to the strong electric field component of the shortest electron bunches. The data analysis showed this anisotropy is strong enough to influence the magnetic switching dynamics and the result is the first proof of principle demonstration of a mechanism for all electric field switching of a thin film metallic ferromagnet at room temperature. Such manipulation of the magnetization is of great interest for not only its fundamental importance to the study of magnetism but also for practical reasons. Primarily, it holds great promise for use in future data storage devices which would write data using only electric fields. This would eliminate the need for the comparatively energetically inefficient magnetic field based switching systems used today.

FY 2009 Authorized Budget (New BA): $424K

Program Personnel Supported in FY2009:

PI:	Stohr, Joachim	5%
PI:	Siegmann, Hans	100%
Student:	Gamble, Sara	100%
Student:	Kukreja, Roopali	83%
Student:	Rick, Ramon	100%

Interactions:

SSRL and the PULSE Institute; Department of Applied Physics, Stanford University; IBM Research Center San Jose, CA 95120; IBM Research, Zurich Research Laboratory, 8803 Ruschlikon, Switzerland; Bogolyubov Institute for Theoretical Physics 14-b, Metrolohichna str., Kiev 03680, Ukraine.

Related Project URL:

FWP Title: "PULSE:The Stanford Photon Ultrafast Science and Engineering Center

Laboratory Name: SLAC National Accelerator Laboratory-PULSE

FWP Number: SCW0063

B&R Code: KC0202010

Program Abstract:

Subtask D.2.b: Energy and angular momentum transfer in solids

We apply different approaches to the question of angular momentum transfer in solids on an ultrafast time scale. The first approach will address the question of how spatially the magnetization disappears after a ferromagnet has been heated by a femtosecond laser pulse. It is completely unknown on which length scale the magnetization gets randomized and which time scales can be associated with the length scales. To answer this question we are employing time resolved coherent soft x-ray scattering at beamline 13 of SSRL. We plan to heat a ferromagnetic thin film deposited on s SiN window by a femtosecond laser pulse. In order to observe nanoscale dynamics we scatter soft x-rays on the magnetic structure.

Another point of view on ultrafast demagnetization focuses on the problem of angular momentum transfer from the spin system to the lattice. It is still unknown how microscopically the angular momentum of the spins can be coupled to the lattice on a femtosecond time scale as the spin orbit interaction in a ferromagnetic solid is small. We are preparing an experiment to observe the demagnetization process by spin resolved photoemission. The sample will be heated by a femtosecond laser pulse and the sample will be probed by the x-ray pulse from a free electron laser. We intend to do this experiment at LCLS as well as FLASH in Hamburg, Germany

Program Impact:

The preparation of FEL and synchrotron based experiments of this complexity require the collaboration of several PIs. The design and construction of the ultrafast demagnetization experiment at LCLS and FLASH involves the design of spin polarization conserving electron optics, sample fabrication chambers, electronics and a spin detector. The task goes beyond the capabilities of a single investigator. The scope of this task is strongly connected to accelerator based x-ray sources which require the expertise available at national labs.

FY 2009 Authorized Budget (New BA): $491K

Program Personnel Supported in FY2009:

PI	Y. Acremann	(75%),
PI	A. Lindenberg	(30%)
PI	J. Stohr	(5%)
Research Associate	Scherz, Andreas	(25%)
Student	D. Zhu	(100%),
Student	R. Kukreja	(17%)
Student	T. Wang	(25%)

Interactions:

We collaborate with the group of Prof. Kelly Gaffney (PULSE) for lab based laser experiments. The laser for the SSRL based pump-probe experiment is used in collaboration with Prof. Aaron Lindenberg (PULSE). Dr. Andreas Scherz (SIMES) is in charge of the SSRL based coherent scattering experiment. Dr. Olaf Hellwig (Hitachi) is preparing samples.

The electron optics of the time resolved photoemission experiment is currently being developed at ETH Zurich in collaboration with Prof. Andreas Vaterlaus and Prof. Danilo Pescia. The experimental setup at FLASH is currently being designed together with Prof. Wilfried Wurth at DESY as well as Prof. Alexander Föhlisch at BESSY.

FWP Title: "PULSE:The Stanford Photon Ultrafast Science and Engineering Center

Laboratory Name: SLAC National Accelerator Laboratory-PULSE

FWP Number: SCW0063

B&R Code: KC0202010

Program Abstract:
Subtask D.2.d: Magnetic Material Research
The goal of this program is to understand the interaction with ultrafast, intense soft x-ray pulses from a free electron laser (FEL) with materials and especially magnetic materials. While FEL applications will clearly break new scientific ground across scientific disciplines, possibly the most important question regards the utility of FELs for studies of the electronic structure of materials, whose understanding drives progress in key areas of societal importance like energy, the environment and technology.

This program is first aimed at demonstrating the feasibility of spectroscopy using XFELs. While at conventional synchrotron radiation sources energy selection and tuning are accomplished by a monochromator, the intrinsic spectrum of an x-ray free-electron laser FEL is ill suited for such measurements. Based on the self-amplified spontaneous emission SASE process of FELs, the photon spectrum is peaked at an energy and stochastically fluctuates shot-to-shot by an amount comparable to the energy width of each single pulse. Hence, if a monochromator is used to control the excitation energy, the intensity greatly fluctuates and may even be zero for certain pulses. This leads to severe intensity normalization problems. These problems have been solved by the use of a unique sample geometry that captures as much information as possible on a shot-by-shot basis. A post-data collection normalization scheme was also developed to deal with the severe non-linearities in the detection apparatus.

Our program is also aimed at addressing the fundamental question of under which conditions an XFEL pulse can be expected to act as a weak perturbation as for present storage-ring based x-ray sources, and when the x-ray perturbation will lead to radically altered electronic states. In the latter case, the information on the as-prepared state of the sample would be lost, preventing one from obtaining the desired electronic structure information. The results of the proposed program are therefore of key importance for the applicability of the new generation of FEL sources for materials science, in general, and magnetism research, in particular.

This program is has now been closed.

Program Impact:
This program is a collaboration between PULSE PI's Joachim Stohr, Andreas Scherz and Yves Acremann, as well as DESY PI's Wilfred Wurth and Alexander Föhlisch. The experiment measurements for this project were performed at FLASH in Hamburg. It was therefore essential to combine the knowledge of the FLASH machine and preparations in Germany with sample preparations and data analysis at SLAC.

FY 2009 Authorized Budget (New BA): $203K

Program Personnel Supported in FY2009:

Research Associate:Braeuer, Bjoern 30%
Research Associate: Sarkar, Shampa 75%
Student: Burkhardt, Mark 75%
PI: Stohr, Joachim 5%

Interactions:
External: Prof. W. Wurth, DESY (Germany), Prof. Alexander Föhlisch
Internal: Yves Acremann (PULSE) and Andreas Scherz (SIMES) who collaborated on the experiments.

FWP Title: "PULSE:The Stanford Photon Ultrafast Science and Engineering Center

Laboratory Name: SLAC National Accelerator Laboratory-PULSE

FWP Number: SCW0063

B&R Code: KC0202010

Program Abstract:
Subtask D.3.a: THz and strong field nonlinear spectroscopy and control of material structure

Program explores the nonlinear properties of materials induced by strong fields. Special concentration is the nonlinear transient changes in materials exposed to strong and ultrafast electromagnetic fields, such as the THz fields of relativistic electron beams, as well as the strong fields of focused laser beams. Research advances are directed towards materials and x-ray science of coherent phonons in materials exposed to THz pulses; nonlinear excitation of coherent phenomenal in materials; field-induced effects in materials; transient phase changes in materials; transient domain creation and motion in materials. Reis became PI of this subtask as of January 2009 and scope has been expanded to include momentum and time-resolved nonequilibrium phonon dynamics**.**

Program Impact:
This program currently concentrates on nonequilibrium dynamics in solids with atomic-scale resolution in time and space and with atomic specificity, as well as on the strong-field response of materials to electromagnetic radiation. As it studies fundamental properties of matter on the fastest time scales and shortest distances it is of direct interest tot eh DOE-BES mission. It makes use of state of the art x-ray facilities within the DOE complex, including SSRL and the APS, and will soon make use of LCLS. The highly collaborative structure of PULSE provides collective expertise in ultrafast laser and x-ray science, condensed matter and materials physics.

FY 2009 Authorized Budget (New BA): $331K

Program Personnel Supported in FY2009:

Student:	Chen, Jian	50%
Student:	Cryan, James	8%
Research Associate:	Ghimire, Shambhu	50%
Student:	Hassan, Vinayak	17%
PI:	Reis, David	72%

Interactions:
External Collaboration with Rob Henning and Tim Graber, U. Chicago/BioCars APS
External Collaboration with Stephen Fahy, University College Cork
External Collaboration with Lou DiMauro, Ohio State
External Collaboration with Roberto Merlin, University of Michigan

Related Project URL:

FWP Title: "PULSE:The Stanford Photon Ultrafast Science and Engineering Center

Laboratory Name: SLAC National Accelerator Laboratory-PULSE

FWP Number: SCW0063

B&R Code: KC0202010

Program Abstract:
Subtask : D.3. b "Laboratory-based THz pump experiments"

A laboratory-based source for intense, ultrashort THz radiation is applied to investigate and control the electronic and structural properties of materials under intense electric and magnetic fields. We seek to develop the field of ultrafast nonlinear THz spectroscopy as a new tool in materials science.

Program Impact:

We are developing nonlinear THz spectroscopy as a tool for probing and controlling material properties. Developing methodology for all-optical electric field and vibrational control of material structural and electronic dynamics, including ferroelectric materials, semiconductors, and nanoscale materials. We have also been investigating mid-IR vibrational excitation of liquid phase dynamics probing using ultrafast x-ray techniques. This program lays a foundation for future THz-based experiments using ultrafast electron bunches produced by the linear accelerator at SLAC and for THz-pump/X-ray probe experiments at the LCLS.

FY 2009 Authorized Budget (New BA): $171K

Program Personnel Supported in FY2009:
PI: Aaron Lindenberg (20%)
Research Associate: Haidan Wen (100%)

Interactions:
Internal—Stanford Materials Science and Engineering Dept., Stanford Synchrotron Radiation Laboratory
External—Advanced Light Source at Lawrence Berkeley National Laboratory, Advanced Photon Source at Argonne National Laboratory, Materials Science Division at Argonne National Laboratory.

Related Project URL: