2012-2013





INSTITUTE FOR TERAHERTZ SCIENCE AND TECHNOLOGY

Annual Report



Dr. Mark Sherwin, Director | Marlene Rifkin, Business Officer Website: http://www.itst.ucsb.edu | marlene@itst.ucsb.edu

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Mission Statement

The mission of ITST is to

advance science and technology at the heart of the electromagnetic spectrum* while training and inspiring new generations of scientists, engineers, and the public at large and supporting research with outstanding service in a warm, welcoming and fun workplace.



Figure 1: Chart showing ITST's research emphasis at the heart of the electromagnetic spectrum.

*roughly 0.1-10 terahertz (1 terahertz= 10^{12} cycles/s). For reference, cell phones transmit near 1 GHz (10^{9} cycles/s) and the spectrum of visible light stretches from about 400-800 terahertz.

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Director's Statement

The heart of the electromagnetic spectrum—between 0.1 and 10 terahertz—is home to 98% of the photons in the universe. It is thus not surprising the astrophysicists pioneered the development of terahertz technology. Within the last 20 years, terahertz science and technology have been growing vigorously here on earth. The Institute for Terahertz Science and Technology (ITST) at UC Santa Barbara is internationally known as a leading center for terahertz research.

In March of this year, the Planck space mission released the most accurate and detailed map ever made of the oldest light in the universe—terahertz light-- revealing new information about its age, contents and origins. Planck is a European Space Agency mission with significant participation by ITST researchers Phil Lubin, Peter Meinhold and Jatila van der Veen. Water vapor in the atmosphere heavily attenuates many frequencies of terahertz radiation, which is why Planck made its observations from space. However, astrophysical observations from the earth's surface are possible from locations that are sufficiently high and dry. The map on the cover of the annual report was generated by ITST graduate student researcher Jon Suen from the experimental cosmoloty group led by Phil Lubin. The regions in dark blue are sufficiently dry to be interesting sites for terahertz telescopes. Many of the sites that Jon found in his survey were known, and house existing telescopes—Antarctica and the high Andes, for example. Jon discovered that Tibet would also be an excellent site—and it is accessible by train, which cannot be said of any of the other dark blue sites.

Right here at UCSB, the world's brightest sources of tunable terahertz radiation—the UCSB Free-Electron Lasers—yielded a breakthrough in the field of magnetic resonance, which was reported in September 2012 in the journal *Nature*.¹ For the first time, a free-electron laser was used to power an electron paramagnetic resonance (EPR) spectrometer. EPR is a cousin of the more famous and familiar nuclear magnetic resonance (NMR), and magnetic resonance imaging (MRI). Whereas NMR and MRI operate on atomic nuclei, EPR operates on electrons. Each electron can be thought of as a tiny magnet that senses the magnetic fields caused by atoms in its nano-neighborhood. With FEL-powered EPR, we have shattered the electromagnetic bottleneck that EPR has faced, enabling electrons to report on faster motions occurring over longer distances than ever before. We look forward to breakthrough science that will lay foundations for discoveries like new drugs and more efficient plastic solar cells. The development of FEL-powered EPR was supported by funds from the NSF and the W. M. Keck Foundation.

We have also taken an important step to increase the impact ITST's unique facilities on research at UCSB and beyond—we ran an international search for a Principal Experimentalist at ITST. We hired Dr. Nikolay Agladze, a virtuoso experimentalist with deep and broad experience in terahertz spectroscopy and instrument building. He is available to assist any researcher with experiments at ITST. We will talk more about him in the next annual report.

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Organizational Chart



Advisory Committee

Songi Han

Chemistry and Biochemistry, Committee Chair

S. James Allen Andrew Cleland Ben Mazin Christopher Palmstrom Kevin Plaxco Luke Theogarajan Win Van Dam Former iQuest Director, Physics Physics Physics Electrical and Computer Engineering Chemistry and Biochemistry Electrical and Computer Engineering Computer Science

Ex Officio Members

Omer Blaes Rick Dahlquist Marlene Rifkin Mark Sherwin Chair, Physics Chair, Chemistry and Biochemistry Business Officer, ITST Director, ITST, Physics

Personnel

Administrative Staff-ITST

Marlene Rifkin, Business Officer Rita Makogon Contract and Grant Manager Rob Marquez Contract and Grant Analyst Elizabeth Strait Computer and Network Administrator

Technical Staff-ITST

David Enyeart Senior Development Engineer Aaron Ma Junior Development Engineer Gerald Ramian Research Specialist Emeritus

¹ Takahashi, S.; Brunel, L. C.; Edwards, D. T.; van Tol, J.; Ramian, G.; Han, S.; Sherwin, M. S., Pulsed electron paramagnetic resonance spectroscopy powered by a free-electron laser. *Nature* **2012**, *489*, 409-413;

Other Project and Activities

Seminars and Workshops

ITST continued its very successful lunchtime Seminar Series. Refreshments (usually pizza) were provided. The following seminars took place throughout the year:



¹ Takahashi, S.; Brunel, L. C.; Edwards, D. T.; van Tol, J.; Ramian, G.; Han, S.; Sherwin, M. S., Pulsed electron paramagnetic resonance spectroscopy powered by a free-electron laser. *Nature* **2012**, *489*, 409-413;

12/18/12:

Terahertz Devices Built on 2DEGs: Huili (Grace) Xing, Electrical Engineering Department, University of Notre Dame

01/10/13:

Frontiers in Terahertz Science: Mark Sherwin, ITST, Physics Department, University of California, Santa Barbara

01/17/13:

Light Induces Degradation of Thin-Film Silicon Solar Cells Studied by Multi-Frequency EPR: Matthias Fehr, Department of Chemistry and Biochemistry, University of California, Santa Barbara

01/31/13:

Self-Assebled ErSb Nanostructures of Tunable Shape and Orientation: Hong Lu, Materials Department, Daniel Ouellete, Physics Department, Justin Watts, Physics Department, University of California, Santa Barbara

02/14/13:

The Chemotaxis Signaling Complex: Frederick Dahlquist, Department of Chemistry and Biochemistry, University of California, Santa Barbara

02/21/13:

The EPR-FEL: Gerald Ramian, ITST, University of California, Santa Barbara

03/07/13:

Developing Ultrafast Electron Paramagnetic Resonance at 240 GHz: Devin Edwards, ITST, University of California. Santa Barbara

03/14/13:

Unpaired Spins in Very Low Bandgap Conjugated Polymers and Small Molecules: Fred Wudl, Department of Chemistry and Biochemistry, University of California, Santa Barbara

04/11/13:

Low Energy Modes in Crystalline Solids: Ram Seshadri, Materials Department, Department of Chemistry and Biochemistry, Materials Research Laboratory, University of California, Santa Barbara

04/18/13:

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Direct Measurement of Triplet Exciton Diffusion Length in Organic Semiconductors: Oleksandr (Alex) Mikhnenko, Department of Chemistry and Biochemistry, University of California, Santa Barbara

4/25/13:

Water, Water Everywhere: Long-Distance THz Transmission from the Driest (and notso-dry) Places on Earth: Jon Suen, Experimental Cosmology Group, University of California, Santa Barbara

05/02/13:

Optically-Driven Dynamic Nuclear Polarization in Diamond: Jonathan P. King, Eric Scott, Department of Chemistry, University of California, Berkeley, Melanie Drake, Jeffrey a. Reimer, Department of Chemical and Biomolecular Engineering, University of California, Berkeley

05/0/13:

Silver Halide Photonics for Sensing and Detection in the Mid-Infrared: Tomer Lewi, School of Physics and Astronomy, Tel Aviv University

06/06/13:

At the Crossroads of Instrumentation and Experimental Physics: Nick Agladze, Laboratory of Atomic and Solid State Physics, Cornell University

06/10/13:

In Situ Electron Paramagnetic Resonance Capabilities: Continuous Flow, High Pressure and Electrochemistry: Eric Walter, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory

06/13/13:

Experiments and Diagnostics for Intense Beam Focusing: Prabir Roy, Lawrence Berkeley National Laboratory, University of California, Berkeley

06/21/13:

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Cryogen-Free THz Detection and Imaging: Ken Wood, QMC Instruments Ltd., School of Physics & Astronomy, Cardiff University, UK

Awards Administered

(July 2012 – June 2013)

NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

Guenter Ahlers National Science Foundation, DMR-0702111 Turbulent Convection in a Fluid Heater from Below 05/01/07-04/30/13 \$775,000

Turbulent convection in a fluid heated from below occurs naturally in Earth's atmosphere and oceans where it influences climate and weather, in Earth's mantle where it contributes to the motion of continental plates, in Earth's outer core where it determines the magnetic field, in the Sun where it influences the temperature on Earth, and in many industrial processes where it may have significant economic consequences. This grant supports experiments under highly controlled laboratory conditions and in samples of idealized shapes where some of the central physical components of this process can be studied quantitatively. These components include relatively quiet fluid layers just above the bottom and below the top plate (the "boundary layers"), and a turbulent interior with highly fluctuating temperature and fluid-flow. A large convection cell, known as the "wind of turbulence", is superimposed on these interior fluctuations. Quantitative measurements will be made of the turbulent enhancement of the heat transport, of the temperature distribution in the interior, and of the wind dynamics. The highly quantitative experiments are of modest complexity and thus afford an exceptional diverse learning experience for both graduate and undergraduate students who participate in the work.

Guenter Ahlers National Science Foundation, DMR-1158514 Turbulent Convection in a Fluid Heated from Below 06/01/12-05/31/16 \$320,000 (640,000)

Turbulent convection in a fluid heated from below is of utmost importance in many natural phenomena and in industry. It occurs in Earth's mantle where it contributes to the motion of continental plates and influences vulcanism. In the outer core of the Earth it determines the magnetic field in which we live. It is the important heat-transport mechanism in the outer layer of the Sun and thus impacts the temperature of our environment. It plays a significant role in many industrial processes, where its enhancement or inhibition may have significant economic consequences. These applications range from miniature heattransport devices in computer applications to the giant cooling systems of power plants. And yet much

10 NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

remains unknown to the scientist and engineer about these processes. The proposed work will extend our understanding of turbulent convection to fluids with properties similar to the Earth's atmosphere; this property range has remained relatively unexplored in the laboratory. The work will also be extended to samples that are rotated about their vertical axis. The rotation will exert a force on the fluid known as the Coriolis force and thus will change the behavior of the system in a manner related to how Earth's rotation modifies the nature of hurricanes and ocean currents. These experiments require the construction of complex apparatus and the automatic computer-control of numerous intricate processes. Thus they are an exceptionally good training ground for our young coworkers, many of whom will evolve into the leaders of the next generation of scientists and engineers.

Dirk Bouwmeester National Science Foundation, PHY-0804177 Quantum States of OptoMechanical Structures 08/01/08-07/31/12 \$600,000

Quantum theory has been extremely successful in explaining many aspects of the world around us. Despite this achievement, fundamental aspects of the quantum theory are as mysterious as they were to the founders of the theory. Especially remarkable is the feature that a particle somehow obtains information about different "paths" it could have taken. This observation leads to the question of what would happen if such quantum effects could be observed in macroscopic objects. If the laws of quantum mechanics remain valid for large objects, one seems to be forced to accept that cats can be alive and dead at the same time (following Schroedinger's famous thought experiment). However, others question whether such a drastic conclusion is justified based on the current support for the theory. The fact is that all experiments to date that directly tested the quantum superposition of individual objects are restricted to photons, atoms, molecules and ensemble of electrons. Furthermore the quantum theory is faced with problems when trying to unify it with the theory of relativity. It is not possible either on theoretical or experimental grounds, therefore, to rule out the possibility that quantum mechanics does not apply to large objects. Optical technology has progressed to the level that it is conceivable to put a small mirror into a superposition of two quantum states. The experiment will be done with a particularly tiny mirror, smaller in diameter than a human hair but still about ten billion times more massive than any object previously brought into a quantum superposition. This award provides support for the mirror and cantilever fabrication as well as for designing a liquid-helium cooled apparatus and performing supporting theoretical work. Furthermore it provides travel support for establishing a close collaboration with international experts on sub-millikelvin systems. Testing quantum mechanics in this unexplored regime is first of all of fundamental importance. The optical control of micro-mechanical systems, in particular the application of optical cooling techniques, is however also expected to be of broad interest in metrology and could also be used for several different experiments such as generating squeezed light and resonance enhanced Casimir forces. This research program involves significant educational component, and the research is excellent for teaching fundamental properties of quantum mechanics and micro-mechanical systems and for training young researchers in state-of-the-art technologies in a multidisciplinary and international environment.

Dirk Bouwmeester Pierre Petroff National Science Foundation, ECCS-0901886 Solid State Cavity Electrodynamics 06/03/09-08/31/12 \$399,914

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

The objective is to develop solid-state devices for achieving controlled and efficient coupling between single photons and single electrons confined in microstructures.

Dirk Bouwmeester Elisabeth Gwinn Deborah Fygenson Everett Lipman Michael Liebling National Science Foundation, DMR-0960331 MRI-R2 Nano Photonic Imaging System 03/15/10-09/20/13 \$464,703

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

A rapidly expanding field of research concerns the development of new techniques for optical imaging of nanometer to micron scale structures, such as biological molecules with integrated functional elements, semiconductor optoelectronic devices and cells. The investigator team proposes to develop an unconventional optical instrument capable of resolving structures on the scale of a few tens of nanometers, by using special correlated states of light (such as entangled two-photon states) in combination with an ultra stable optical platform with nanometer resolution scanning capabilities and recently-developed signal processing algorithms. In order to probe the special light-matter interactions that occur when phonon-induced dephasing is minimal, the system is designed to operate at cryogenic as well as ambient temperatures. The wide wavelength range of this nano-photonics imaging system would enable investigation of structures ranging from semiconductor nanodevices to DNA scaffolds to living cells. The research team consists of experts in the key technological aspects: quantum optics, high resolution optical imaging and high speed image processing, ultra-low vibration and low-temperature operation, and biological system design.

Dirk Bouwmeester National Science Foundation, PHY-1206118 Quantum Post-Selected Optomechanics 09/01/12-08/31/16 \$220,000 (\$670,000)

This proposal is the result of an analysis of the currently limiting factors in achieving macroscopic superpositions of optomechanical systems. We propose a new scheme based on quantum post-selection that will remove two of the main limitations of the current approaches. With the implementation of this new scheme together with proposed advances in the design and fabrication of optomechanical systems (based on the use of Graphene, Boron Nitride and Carbon nanotube technology) we expect to make very significant progress towards testing quantum mechanics at the macroscopic scale.

Michael Bowers UC Los Angeles, SB070075 Pathogenic Protein Folding and Human Disease 09/01/06-07/31/12 \$1,292,132

The objective of this research is to understand, on a molecular level, the folding and assembly of Aβprotein alloforms. Recent results indicate small. Soluble oligomers of Aβ are responsible for initiating a pathological cacadw resulting in Alzheimer's disease (AD). Aβ42 has been shown to be the primary neurotoxic agent even though Aβ40 is nearly 10 times more abundant, Single-point amino-acid substitutions at positions 22 and 23 in Aβ42 account for a variety of familial forms of AD. It is our hypothesis that Aβ monomers and small oligomers are important therapeutic targets and characterization of their structure and mechanisms of folding and assembly are critical research objectives. Here we propose to apply, for the first time, the powerful methods of ion mobility spectrometry coupled with mass spectrometry (IMS-MS) to the problem of Aβ folding and assembly. These methods provide accurate measures of monomer and oligomer cross sections and oligomer size distributions. When coupled with high-level molecular dynamics modeling, monomeric structure with atomic detail is obtained. The method is ultrasensitive, routinely working with picomoles of sample or less. These methods can be readily extended to other neurological diseases like ALS and Parkinson's disease that share the misfolding/aggregation motif with AD.

The specific aims of this research are (1) to structurally characterize $A\beta$ monomers and to determine how these structures change with single-amino-acid substitution, oxidation or other simple sequence modification, (2) to structurally characterize $A\beta$ monomer fragments and determine how these structures change with sequence length, single-amino-acid substitutions or other modifications, and (3) to measure oligomer-size distributions and oligomer structures for the early stages of assembly if $A\beta$ and modified forms of $A\beta40$ and $A\beta42$.

Michael Bowers National Science Foundation, CHE-0909743

13 NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

Non-Covalent Complexes 08/01/09-07/31/13 \$730,000

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

In this award funded by the Experimental Physical Chemistry Program of the Division of Chemistry, Professor Michael Bowers of University of California, Santa Barbara, explores the question of why peptides and proteins in living systems are solely composed of L-amino acids - one of the deepest mysteries in biology. Professor Bowers and his students will start with several simple model systems of peptides that are available in a wide range of chirally mixed forms. These peptides are small enough (5 or 6 amino acids long) that good theory can be done on them to help understand observed changes in their folding and aggregation tendencies as a function of their chiral purity. These peptide families will also provide an entrée into a second major thrust of the proposal - amyloid formation mechanisms. Amyloids are ubiquitous in complex living systems and are implicated in many serious diseases (Alzheimer's, type 2 diabetes, etc.). The goal is to understand the aggregation process and how initially coiled or alpha-helical oligomeric systems end up as large beta-sheet assemblies. As part of this effort Professor Bower's team will initiate a collaboration with Gerhard Meijer and Gert Von Helden at the Fritz Haber Institute in Berlin. This group is building a state of the art instrument to Professor Bower's specifications for this work to couple with a new free electron laser under construction at that facility. Finally the researchers have initiated studies on a related biologically important amyloid system, the 37 residue IAPP or amylin peptide, involved in type 2 diabetes. The human wild type peptide rapidly forms large oligomers but a number of very similar peptides do not. Preliminary data implicate compact assemblies as leading to fibril formation (and hence disease) while elongated assemblies of the same oligomer number do not aggregate further. Modeling and further experiments are planned to fully understand these initial results.

Science education in the United States is in a sustained downturn that threatens our world leadership in both innovation and technology development. The problems start early. The 5th grade has been targeted as the first "go" or "no go" indicator in a child's scientific development. At UCSB there is a strong outreach program at the 5th grade level initiated and sustained by a former group member with continuing help from current research group members. Professor Bowers decided to tackle the second "go" or "no go" decision time in young adults - their high school years. His group is developing an outreach program using all group members to present their research projects to high school classes and to relate their personal scientific stories and how they ended up in graduate school at UCSB. A preliminary trial with one of the group members has been run with encouraging results. Additional UCSB faculty and research groups will be incorporated as the program grows.

Michael Bowers Air Force FA9550-11-1-0113 Litigated Metal Clusters: Structures, Energetics and Reactivity 06/15/11-06/14/14

14 NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

\$380,000 (\$570,000)

The field of metal clusters, their reactivity and ligand binding energies has undergone a renaissance in recent years. There are two principle drivers: The importance of metal clusters in catalysis and their fundamental importance as bridging agents between the atomic and the solid phases of matter. The Bowers group is uniquely positioned to contribute to this important area of research. They have developed two tools that allow structural determination for size-selected clusters: ion mobility methods that yield accurate cross sections and sequential ligand binding energies that identify equivalent binding sites. These have been applied primarily to coinage metals but here the group will extend these studies to transition metal clusters.

Michael Bowers Asian Office of Aerospace R&D, FA2386-12-1-3011 Metal and Litigated Metal Clusters: A New Instrument 7/1/12-01/11/14 \$269,309

A request is made is transform a currently existing instrument onto one capable of studying massselected metallic and litigated metal clusters. The makeover will require a new cluster source, a new temperature-dependent ion mobility and reaction cell, and several upgrades to the current ion optics. A new laser will be required to generate the clusters. The focal point of the work will be determination of cluster structure and reactivity. The instrument will take advantage of novel structural methods we have developed based on ligand binding energies and entropies as well as ion mobility cross sections. Finally, new work is proposed for metal oxide clusters where the structural methods developed here have yet to be applied.

Steven Buratto Michael Bowers Horia Metiu National Science Foundation NSF CHE-1152229 Model Nanocluster Catalysts: The Role of Size, Shape and Composition on the Catalytic Activity of Small Metal Oxide and Bimetallic Clusters on Oxide Surfaces 04/01/12-03/31/15 \$450,000

A large number of industrial processes use nanometer-size clusters (both metal and metal oxide) supported on oxide surfaces to perform reactions that would not take place, or would be commercially unsuccessful if performed on the bulk material. In research supported by this grant the investigators will utilize state-of-the-art experimental and theoretical methods to probe the catalytic activity of well-defined nanocluster catalysts in great detail and develop a fundamental understanding of the catalytic

chemistry at the atomic level. The concepts developed through this research will help optimize important industrial processes using these nanoscale catalysts and provide valuable insight into the discovery of new nanoscale catalytic materials. Researchers supported by this grant will also be active in outreach to K-12 schools in the Santa Barbara area. They plan to develop a tutorial presentation on an atomistic view of heterogeneous catalysis that will be included in the currently active outreach program in the department at UCSB. In addition, researchers working on this project will visit high schools in the Santa Barbara and Ventura Counties three times per year to discuss their research and its impact as well as to promote science education.

Steven Buratto National Science Foundation NSF CHE-1213950 Connectivity and ION Conductance in Field Cell Membranes Probed by Tunneling Atomic Force Microscopy 07/01/12-06/30/15 \$283,864

Proton exchange membrane (PEM) fuel cells, which convert chemical energy into electricity using an electrochemical cell, could be used as efficient power sources, offering high power density and low environmental impact. Critical to PEM fuel cell performance is the polymer electrolyte, which is an efficient proton conductor but electric insulator. The most common PEM material is the polymer electrolyte Nafion®, which is composed of a hydrophobic Teflon® backbone and side chains terminated with hydrophilic sulfonic acid (SO₃H) groups. In a Nafion® film the hydrophilic pores, which conduct protons, form via phase separation of the side chains from the polymer backbone. The proton conducting channels in these films are strongly dependent on the film morphology and the environmental conditions. A detailed understanding of proton conduction, in terms of the size and distribution of the chemical domains responsible for transport, is central to both a complete understanding of fuel cell performance and a systematic approach to improving the performance. Toward this end, conductive atomic force microscopy (cAFM) will be used to gain a fundamental understanding of ion conduction in proton exchange membrane fuel cells. Using the nanoscale resolution afforded by cAFM, the size, spatial distribution, and electrochemical activity of ion transport domains in polymer electrolytes will be explored under operation fuel cell conditions.

David Cannell National Aeronautics and Space Administration, NNX08AE53G Gradient Driven Fluctuations 03/01/08-08/31/12 \$190,000

This research continues the work done previously. Although we do not yet have the data in hand, our experiment was flown aboard the Foton-M3 mission on September 14-26, 2007. Hopefully, our results

16 NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

will provide insight into the behavior of single-component fluids and mixtures, including protein solutions, when placed in the microgravity environment, and subjected to temperature and/or concentration gradients. This might be of considerable interest to anyone attempting crystal growth in the microgravity environment, for example, because the growth process of necessity generates concentration gradients, and thus enhanced fluctuations.

Songi Han Frederick Dahlquist Mark Sherwin Louis-Claude Brunel Johan van Tol National Science Foundation CHE-0821589 MRI: Development of a 240 GHhz Pulsed Electron Paramagnetic Spectrometer with Nanosecond Time Resolution 08/01/08-07/31/12 \$1,254,623

The Department of Chemistry and Biochemistry at the University of California-Santa Barbara will develop a 240 GHz pulsed electron paramagnetic resonance spectrometer (EPR) with this award from the Major Research Instrumentation (MRI) program. This high frequency EPR spectrometer will capitalize on the tunable terahertz excitation pulses generated at UC Santa Barbara's Free Electron Laser (FEL) facility. The instrument will push the frontier of EPR spectroscopy to more than twice the current frequency/field limitation. It will open up new areas of investigation of the structure and dynamics in biological, chemical and electronic systems.

EPR spectroscopy detects changes in electron spin in materials that contain an unpaired electron. This provides information on the structure and motions of the material at an atomic level. The resultant data provides insight on the properties of materials such as proteins, enzymes and defects in solid materials. This new instrument will allow the study of proteins in biologically relevant environments that were heretofore impossible in many cases. After development, the new spectrometer is intended to become a multi-user facility because of its unique capabilities. Graduate and undergraduate students will be involved in this project learning skills in the design and construction of state-of-the-art instrumentation.

Bruce Lipshutz National Science Foundation, CHE-0937658 EAGER: Chemistry of Water-Intolerant Intermediates....in Water 09/01/09-08/31/12 \$200,000 This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

This project will initiate work on the development of methods for two unprecedented reactions: (1) in situ Grignard formation and use in cross-coupling reactions in water, and (2) formation of unstabilized ylides for Wittig-like olefinations, also in water. These will take advantage of micellar catalysis, where the reactive species to be generated either on the surface of the metal, or within a micelle, are protected from their aqueous surroundings by the hydrophobic interior of these nanoparticles. For these studies, many variables will need to be screened, including the nature of the amphiphile that is to supply a dry reaction medium, in water.

With this award, the Organic and Macromolecular Chemistry Program is supporting the research of Professor Bruce H. Lipshutz of the Department of Chemistry at the University of California, Santa Barbara. Professor Bruce Lipshutz's research efforts revolve around the development of new synthetic methods for the formation of C-C, C-H, C-O, and C-N bonds. Such chemistry will contribute to environmentally benign methods for chemical synthesis, as these new processes will be developed in the absence of organic solvents. Successful development of the methodology will have an impact on synthesis in the pharmaceutical, fine chemicals, and agricultural industries.

Bruce Lipshutz National Science Foundation, CHE-094879 New Technologies Based on Organocopper Catalysis 06/01/10-05/31/13 \$489,000

This project will explore several synthetic methods that rely on copper as the metal that effects catalysis. A number of the transformations are on copper hydride chemistry, which includes new uses of nonracemically ligated CuH for syntheses. The potential to realize unprecedented ligand-accelerated catalysis with CuH in pure water at room temperature will be pursued, along with the potential to deliver water-sensitive carbon-based residues via conjugate addition chemistry, with both approaches based on micellar catalysis in water. Heterogeneous processes that take advantage of both readily accessed valence states of copper [Cu(I) and Cu(II)] impregnated into the pores of inexpensive charcoal matrices will also be developed. A high substrate-to-ligand ratio and tandem processes that can be carried out in a single reaction vessel will be studied.

With this award, the Chemical Synthesis Program is supporting the research of Professor Bruce H. Lipshutz of the Department of Chemistry at the University of California, Santa Barbara. Professor Lipshutz's research efforts revolve around the development of organocopper-based asymmetric catalysis leading to new methods for the formation of C-C and C-H bonds. Such chemistry will contribute to environmentally benign methods for chemical synthesis as most of these new technologies will be developed in the absence of organic solvents, where water serves as the macroscopic medium. Successful applications of the methodology will have an impact on synthesis in the pharmaceutical, fine chemical, and agricultural industries.

Bruce Lipshutz National Institutes of Health, R01 GM086485-04 Transition Metal-Catalyzed Chemistry in Water at Room Temperature 09/01/11-05/31/13 (05/31/15) \$594,822 (1,110,318)

New technologies are to be developed that "get organic solvents out of organic reactions"; that replace traditional processes that use strictly organic media with a "green" alternative: water. These studies are driven by the potential for decreasing the amount of solvent waste, to be carried out by investigating several reactions in water that are important to the pharmaceutical and fine chemical areas. All are to be done at room temperature, and thus, without any investment of energy for either heating or cooling purposes.

Philip Lubin Jet Propulsion Laboratory, JPL1367008 Planck Educational and Public Outreach Effort at UCSB 02/10/09-09/30/13 \$67,700

This award will fund a cosmology summer session that brings in students from a local high school (Dos Pueblos High and perhaps others) and a local community college (Santa Barbara City College). Graduate students, post doc (Rodrigo) Peter Meinhold and Dr. Lubin will orient the students on the Planck mission and relevant science and technology issues, and then the students will work during the summer as a team on various CMB technology programs for a hands-on summer program. We hope to run this program over a six week period each summer.

Douglas Scalapino Oak Ridge National Laboratory, 4000068439 Studies of the Properties of Strongly Correlated Materials 04/14/08-03/31/14 \$693,429

Using recently developed algorithms and new state of the art computer hardware and architecture, we are seeking to understand the properties of strongly correlated electronic materials. Our work is particularly focused on the challenges posed by the high temperature cuprate superconductors. We believe that an understanding of these materials will open an important area of material science and applications.

Mark Sherwin National Science Foundation, DMR-1006603 Quantum Coherence and Dynamical Instability in Quantum Wells Driven by Intense Terahertz Fields 08/15/10-07/31/14 \$560,000

Beginning when early humans harnessed fire for heat and light, the control of electromagnetic radiation has been central to the development of our species. The notion of electromagnetic radiation is nearly 150 years old, proposed by Maxwell in 1865 and demonstrated with the discovery of radio waves in 1866. Radio waves remained largely a laboratory curiosity for nearly 50 years. It is difficult to imagine modern life without radio waves, microwaves, heat, light, and X-rays, which are now all understood to be manifestations of electromagnetic radiation, listed in order of increasing frequency. However, lying between the frequencies of microwaves and heat, stretching from 0.1 to 10 trillion cycles per second (0.1-10 terahertz) is the so-called 'terahertz gap.' Electromagnetic waves exist in this frequency range, but they are extremely difficult to generate and control. This individual investigator award supports a project that will use the world's brightest pulses of terahertz waves, generated by accelerator-driven 'free-electron lasers', to search for new quantum-mechanical phenomena predicted to occur in nanometers-thick semiconductor devices. The semiconductor devices under study are similar to those used to modulate light in fiber-optic communications, and as ultrafast transistors in cellular telephones. This project will support the education of two PhD students, as well as undergraduate and high-school interns. The students will learn the most advanced techniques to generate and manipulate electromagnetic radiation across the electromagnetic spectrum, preparing them for leadership in the nation's scientific and technological workforce, and bringing mankind closer to harnessing terahertz radiation for future technologies.

Mark Sherwin

U.S.-Israel Binational Science Foundation 2010130 Development of Gd³⁺-Based Spin Labels for Probing Structure, Dynamics and Interfaces by Electron Paramagnetic Resonance Techniques 10/01/11-09/30/13 (09/30/15) \$45,880 (93,805)

EPR and DNP (dynamic nuclear polarization) rely on the introduction of spin probes or labels to intrinsically diamagnetic systems and the standard, widely used spin labels are based on the nitroxide group that has a spin, S=1/2. The recent development of high field EPR opens new opportunities in spin labeling by exploiting the unique spectroscopic properties of half-integer high spin systems at high fields that can offer high sensitivity and resolution. The objective of this proposal is to establish a new family of Gd^{3+} (S=7/2)-based spin labels for probing structure, dynamic and interfaces of molecules and materials using EPR and DNP at high magnetic fields. The basic spin physics and dynamics of Gd^{3+} spin labels at high fields must be explored and understood in order to realize their tremendous promise

20 NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

for EPR and DNP. Using a variety of mono- and bis-Gd³⁺ compounds we will measure spin lattice relaxation, phase memory time and spectral diffusion as a function of field (95 and 240 GHz. 3.5 and 8.5T), temperature and Gd³⁺ concentration. Having established a good understanding of the spin dynamics that is needed for the optimum measurements conditions and the design of appropriate Gd³⁺ chelators we will explore Gd³⁺ spin labels for structure determination through Gd³⁺-Gd³⁺ distance measurements and their potential to probe protein dynamics and light triggered conformational changes. Finally, we propose to develop a Gd³⁺ spin label based methodology to study polymer interfaces in systems with nanometer scale heterogeneities and phase boundaries using solid state DNP of ¹H and natural abundance ¹³C NMR at 7T

Mark Sherwin S. James Allen Christopher Palmstrom Thuc-Quyen Nguyen Song-I Han National Science Foundation, DMR-1126894 MRI: Development of a Free-Electron Laser for Ultrafast Pulsed Electron Paramagnetic Resonance 10/01/11-09/30/14 \$992,270

The world's brightest source of tunable terahertz radiation will be developed to manipulate electron spins faster than has ever been possible. This ultrafast spin manipulation will enable pathbreaking studies with applications ranging from development of inexpensive solar cells to understanding how protein molecules fit together and move to regulate the flow of energy, information and matter in living organisms.

Electrons and atomic nuclei both have a property called spin, which makes them behave like (very tiny) magnets. In nuclear magnetic resonance (NMR), which is the basis for magnetic resonance imaging (MRI), a strong external magnetic field aligns nuclear spins, while powerful pulses of radio-frequency electromagnetic radiation manipulate nuclei to discover otherwise invisible information about neighboring atoms. Electron paramagnetic resonance (EPR), in a fashion similar to NMR, uses an external magnetic field to align electron spins (rather than nuclear spins). Typically, pulses of microwave-frequency electromagnetic radiation manipulate these electrons to learn about local environments over larger neighborhoods. EPR becomes even more powerful when extremely high-frequency terahertz is used.

The free-electron lasers (FELs) at the University of California at Santa Barbara (UCSB) are famous as the world's brightest sources of tunable terahertz radiation. Recently, researchers at UCSB demonstrated that one of the UCSB FELs could be used to rotate electron spins 50 times faster than ever before at .25 terahertz. This project will fund the construction of an even more powerful FEL. The new FEL, which will be used by scientists from all over the nation and world, will be 100 times more powerful than the existing one, and will pulse ten times faster, enabling at least 1000 times more rapid acquisition of

²¹ NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

experimental data. The EPR spectrometer powered by this new FEL will create an unprecedented capability to observe the structure and ultrafast dynamics of molecules, materials and devices at nanometer length scales.

Mark Sherwin Jet Propulsion Laboratory-JPL, 1468484 10/16/12-9/30/13 \$120,218

This subcontract entails the design tunable antenna-coupled intersubband terahertz (TACIT) hot-electron mixers, characterization of MBE-grown material for TACIT mixers, fabrication of TACIT mixers using UCSB's NanoTech facility, electrically testing fabricated devices, and comparison of the performance of TACIT mixers with theory.

Mark Sherwin National Science Foundation, MCB-1244651 Robust GD³⁺ -Based Spin Labels for Structural Studies of Membrane Proteins 01/01/13-12/31/15 \$331,810 (\$848,526)

Understanding the structure and functional dynamics of membrane proteins in a life-like environment is one of the grand challenges of biology.

Site-directed mutagenesis and spin labeling (SDSL) combined with electron paramagnetic resonance (EPR) enables quantitative studies of the structure and dynamics of membrane proteins and protein complexes. If two sites are labeled on a protein or protein complex, the distance between them can be measured using EPR. The spin $\frac{1}{2}$ nitroxide moiety forms the basis for nearly all spin labels in use today. The goal of this research is to develop a new class of spin labels that are based on the spin $\frac{7}{2}$ Gd³⁺ ion. The attributes of nitroxide and Gd³⁺ -based spin labels are very different and make them optimal for environments that are largely complementary. In particular, the Gd³⁺ ion, with its paramagnetic core shielded by outer electrons, is less sensitive to its local *chemical* environment than the nitroxide moiety, which is delocalized between nitrogen and oxygen atoms. Unlike for nitroxides, phase memory times and linewidths of Gd³⁺ spin labels are relatively insensitive to nearby protons, enabling them to be useful for cw and pulsed EPR on sites and in environments that are not deuterated. The paramagnetic attributes of the Gd³⁺ ion are particularly favorable at high magnetic fields and frequencies, one of the frontiers of EPR. The development of Gd³⁺ spin labels is expected to enable structural studies under a variety of conditions that are biologically important but difficult or impossible to study with nitroxide spin labels.

Jatila van der Veen Phillip Lubin Jet Propulsion Laboratory, JPL 1388406 The Planck Visualization Project: Education and Public Outreach Effort of the U.S. Planck Mission 10/01/09-03/11/15 \$314,715 (\$443,715)

Planck is a mission to measure the anisotropy of the cosmic microwave background (CMB), sponsored by the European Space Agency (ESA) with significant input from NASA. Launched on May 14, 2009, Planck will measure the sky across nine frequency channels, with temperature sensitivity of 10^{-6} K, and spatial resolution up to 5 arc minutes.

NASA participation in Planck is approved and funded, and is manages by the Planck Project at the Jet Propulsion Laboratory in Pasadena, California. The US Planck project is required by NASA to perform Education and Public Outreach (E/PO) as an integral part of the science development. This award serves at the focal point for the E/PO activities of the US Planck team.

Contracts/Grants Awarded 2012-2013

Asian Office of Aerospace Research and Development

Michael BowersFA2386-12-1-301107/01/2012-01/11-2014\$ 269,309Metal and Litigated Metal Clusters: A New Instrument

Jet Propulsion Laboratory

Mark Sherwin146848410/10/2012-11/30/13\$ 120,218Passively-Cooled, Near Quantum=Limited Heterodyne Detector for Space Applicationsincluding High Resolution Planetary and Cometary Spectroscopy

Philip Lubin02/10/09-09/30/14\$ 11,300136700802/10/09-09/30/14\$ 11,300Planck Educational and Public Outreach Effort at UCSB

Jatila van der Veen

138840610/01/09-09/30/2015\$ 77,185The Planck Visualization Project:Education and Public Outreach Effort of the U.S. PlankMission

Jatila van der Veen 1388406 10/01/09-09/30/2015 \$ 17,000 The Planck Visualization Project: Education and Public Outreach Effort of the U.S. Plank Mission

Jet Propulsion Laboratory Subtotal \$ 261,068

National Science Foundation

Guenter AhlersDMR-115851406/01/12-05/31/16\$ 160,000Turbulent Convection in a Fluid Heated from Below

Steven ButattoCHE-121395007/01/12-06/30/15\$ 283,864Connectivity and ION Conductance in Fuel Cell Membranes Probed by Tunneling Atomic ForceMicroscopy

Dirk Bouwmeester				
PHY-1206118	09/01/12-08/31/16	\$ 220,000		
Quantum Post-Selected Optomechanics				

Mark SherwinMCB-124465101/01/13-12/31/15\$ 331,810Robust Gd3+ -Based Spin labels for Structural Studies of Membrane Proteins

Mark Sherwin DMR-1006603 08/15/10-07/31/14 \$ 135,000 Quantum Coherence and Dynamical Instability in Quantum Wells Driven by Intense Terahertz Fields

National Science Foundation Subtotal \$1,130,674

Oak Ridge National Laboratory (Department of Energy GOCO Operated by UT Batelle, LIC.)

Douglas Scalapino 4000068439 04/14/08-03/31/12 \$ 61,630 Study of the Properties of Strongly Correlated Materials

Douglas Scalapino04/14/08-03/31/14\$ 154,075400006843904/14/08-03/31/14\$ 154,075Study of the Properties of Strongly Correlated Materials

Oak Ridge National Laboratory Subtotal \$ 215,705

U.S.-Israel Binational Science Foundation

Mark Sherwin 2010130 10/01/12-09/30/13 \$ 23,515 Development of Gd3+-based spin labels for probing structure, dynamics and interfaces by electron paramagnetic resonance techniques

Research Support Summary (2012-2013)

			% Total
Federal			
Asian Office of Aerospace Research and			
Development	269,309	14%	14%
Jet Propulsion Laboratory	261,068	14%	14%
National Science Foundation	1,130,674	60%	60%
Oak Ridge National			
Laboratory	215,705	11%	11%
Federal Totals	\$1,876,756	100%	99%
International			
U.SIsrael Binational Science Foundation	23,515	100%	1%
International			
Totals	\$23,515	100%	1%
TOTALS	\$1,900,271		100.00%

Charts and Graphs



Chart 1: Research Support Summary Chart 2012-2013



Chart 2: Federal Research Support Summary Chart



Chart 3: International Research Support Summary Chart



Chart 4: Base Budget and Overhead Generated



Chart 5: Number of Proposals Submitted and Funded



Chart 6: Value of Proposals Submitted and Funded



Chart 7: Number of Awards Administered





Statistical Summary for ITST

2012-2013

1. /	Academi	c personnel engaged in research:	21
	a. h	Professional Desearchers (including Visiting)	7
	D.		7
	с.	Specialists	/
	u.	Postdoctoral Scholars	5
	ਦ f	Postavoluota Scholais	
	1		
2. (Graduate	Students:	52
_	а	Employed on contracts and grants	27
	b.	Employed on other sources of funds	0
	C.	Participating through assistantships	0
	d.	Participating through traineeships	0
	е	Other (specify)	0
		TOTAL	27
3. 1	Undergra	iduate Students:	
	a.	Employed on contracts and grants	7
	b.	Employed on other funds	0
	C.	Number of volunteers, & unpaid interns	6_
		TOTAL	13
4. I	Participat	tion from outside UCSB: (optional)	
	a.	Academics (without Salary Academic Visitors)	2
E (b. Stoff (Uni	Other (City College Student)	3
5. 3	Stall (Un a.	iv. & Non-Univ. Funds): Technical	7
	b.	Administrative/Clerical	3
6.	Seminar	s. symposia, workshops sponsored	
7.	Proposa	ls submitted	34
8.	Number	of different awarding agencies dealt with*	23
9.	Number	of extramural awards administered	25
10.	Dollar v	alue of extramural awards administered during vear**	\$14,207,827
11.	Number	of Principal Investigators***	26
12.	Dollar v	alue of other project awards ****	\$261.433
13.	Number	of other projects administered	9
14.	Total ba	ise budget for the year (as of June 30, 2013)	\$157.786
15.	Dollar v	alue of intramural support	\$707.814
16.	Total as	signed square footage in ORU	7.700
17.	Dollar v	alue of awards for year (08 Total)	\$1.900.271
*	Coun	t each agency only once (include agencies to which proposals have been submitted).	

If the award was open during the year, even if for only one month, please include in total. **

Number of PIs, Co-PIs and Proposed PIs (count each person only once.) Other projects - such as donation, presidential awards, fellowships, anything that isn't core budget, extramural, or intramural. ***

Principal Investigators

Guenter Ahlers	Research Professor	Physics
S. James Allen	Research Professor	Physics
James Blascovich	Professor	Psychological and Brain Sciences
Dirk Bouwmeester	Professor	Physics
John Bowers	Professor	Electrical and Computer Engineering
Michael Bowers	Professor	Chemistry and Biochemistry
Steven Buratto	Professor	Chemistry and Biochemistry
David Cannell	Professor	Physics
Frederick Dahlquist	Professor	Chemistry and Biochemistry
Deborah Fygenson	Associate Professor	Physics
Elisabeth Gwinn	Professor	Physics
Song-I Han	Associate Professor	Chemistry and Biochemistry
Michael Liebling	Assistant Professor	Electrical and Computer Engineering
Everett Lipman	Associate Professor	Physics
Bruce Lipshutz	Professor	Chemistry and Biochemistry
Philip Lubin	Professor	Physics
Peter Meinhold	Associate Researcher	Physics
Horia Metiu	Professor	Chemistry and Biochemistry
Nguyen, Thuc-quyen	Professor	Chemistry and Biochemistry/Center
		For Polymer & Organic Solids
Chris Palmstrom	Professor	Electrical and Computer Engineering
Pierre Petroff	Professor	Materials/Electrical and
		Computer Engineering
Douglas Scalapino	Research Professor	Physics
Joan-Emma Shea	Professor	Chemistry and Biochemistry
Mark Sherwin	Professor	Physics
Luke Theogarajan	Associate Professor	Electrical and Computer Engineering
Jatila Van Der Veen	Research Associate	Institute for Terahertz Science and
		Technology/Lecturer College of
		Creative Studies

Map

