



INSTITUTE FOR TERAHERTZ
SCIENCE AND TECHNOLOGY

Annual Report 2008-2009

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Mission Statement

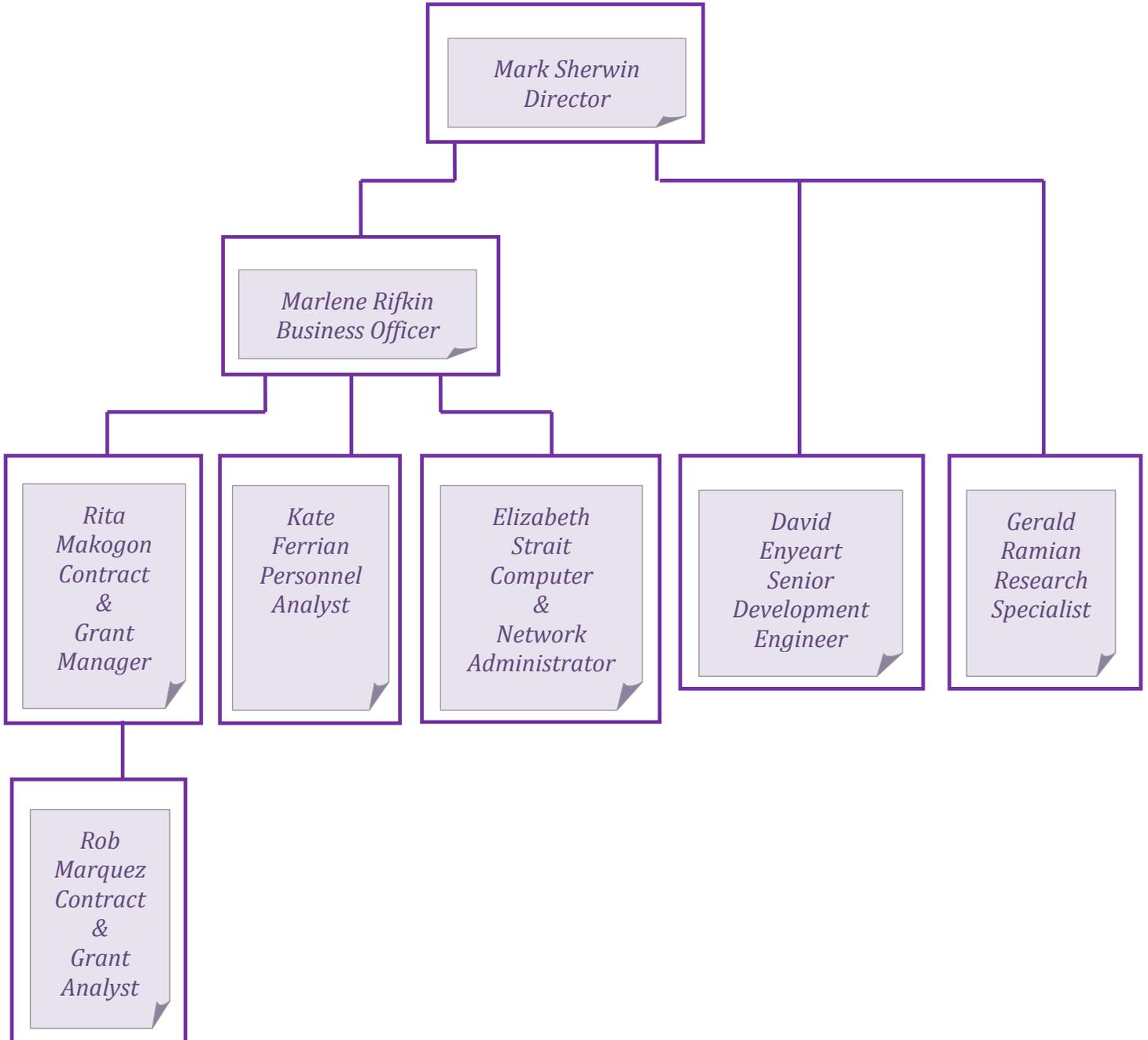
The mission of ITST is to advance science and technology at the heart of the electromagnetic spectrum* while training and inspiring new generations of scientists, engineers, and the public at large and supporting research with outstanding service in a warm, welcoming and fun workplace.



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

3 *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.

Organizational Chart



Advisory Committee

David Stuart	Physics, Committee Chair
S. James Allen	Former iQuest Director, Physics
Elliot Brown	Electrical and Computer Engineering, Materials
Frank Doyle	Chemical Engineering
Art Gossard	Electrical and Computer Engineering, Materials
Songi Han	Chemistry and Biochemistry
Kevin Plaxco	Chemistry and Biochemistry
Ram Seshadri	Materials Department
Joan-Emma Shea	Chemistry and Biochemistry
Chris Van de Walle	Materials Department

Ex Officio Members

Marlene Rifkin	Business Officer, ITST
Mark Sherwin	Director, ITST, Physics
Mark Srednicki	Chair, Physics

Personnel

Administrative Staff-ITST

Marlene Rifkin, Business Officer
Kate Ferrian Personnel Analyst
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
Gerald Ramian Research Specialist

Other Project and Activities

Seminars and Workshops

This year, ITST continued its very successful lunchtime Seminar Series titled “Frontiers in Terahertz Science and Technology”. Refreshments (usually pizza) were provided. The following seminars took place throughout the year:

09/11/08:

Terahertz Technology Based on Low-Dimensional Electronic Devices: Carbon Nanotube Detector and Near-Field Imaging: Yukio Kawano, Riken, Japan. 09/11/08

10/02/08:

A Review: IRMMW-THz 2008 Caltech Sept 15-19:

THz Spectroscopy of Nanomaterials: Mark Sherwin, UCSB

THz Detection with CMOS Arrays: Sangwoo Kim, UCSB

THz Bio Spectroscopy: Jim Allen, UCSB

10/16/08:

Why All the Fuss About Contacts? Making THz Transistors Possible by MBE REgrowth: Mark Wistey, UCSB

10/23/08:

Ultrafast Multiple-Beam Optical and Magneto-Optical Spectroscopy of Selected Centers in Bulk and Nanostructured Si: N. Q. Vinh, FELIX – Free Electron Laser Facility, FOM Institute for Plasma Physics, “Rijnhuizen”, Nieuwegein, The Netherlands.

10/30/08:

Overhauser Spectroscopy of Water: A New Tool to Study Protein Aggregation Kinetics and Membrane’s Fluid Dynamics: Sing-I Han, UCSB

11/06/08:

Self-Assembled Quantum Posts: THz Nanostructures: Christopher Morris, UCSB

12/04/08:

Towards THz Electronics: InP Bipolar Transistors: Evan Lobisser, UCSB

01/15/09:

Towards Nonlinear THz Spectroscopy of Biomolecules: Thomas Feil, UCSB

01/22/09:

Ultrafast Photonics on Semiconducting And Metallic Nanostructures: Markus Betz, Technische Universitat, Munchen, Germany and University of Toronto, Canada

01/29/09:

Photonic Crystal Cavity: A Tool for Studying Strong Interaction of Matter and Radiation in the Terahertz Regime: Cristo Yee, UCSB

02/05/09:

Terahertz Spectroscopy: A New Experimental Probe of Biomolecular Dynamics: Kevin Plaxco, UCSB

02/12/09:

Applications of Spin-Dependent Processes in Semiconductors: Christoph Boehme, University of Utah

02/19/09:

A Level-Set Method for Self-Organized Pattern Formation during Heteroepitaxial Growth: Christian Ratsch, Institute for Pure and Applied Mathematics, UCLA

02/26/09:

Epitaxial Ferromagnetic Metal/compound Semiconductor Heterostructures for Spintronics: Chris Palmstrom, UCSB

03/05/09:

ENDOR and DNP at High Fields and its Relation to Qubit Manipulation: J. van Tol, National High Magnetic Field Lab

03/12/09:

Protein dynamics by Pulsed ESR Spectroscopic Rulers: Sunil Saxena, University of Pittsburgh

04/09/09:

Room Temperature Terahertz Detection with bulk electron plasmon in GaAs Field Effect Transistors: Sangwoo Kim, UCSB

04/23/09:

Optimal Control of Spin and Pseudo-Spin Systems: Steffen J. Glaser, TU Muenchen

04/30/09:

Quantum Coherence in an Optical Modulator: Ben Zaks, UCSB

05/07/09:

Exploring Radicals in Enzymatic Reactions by EPR: Stefan Stoll, UC Davis

05/21/09:

THz Cosmology: Philip Lubin, UCSB

05/28/09:

Investigation of Photoelectrocatalytic Chemical Generation by Semiconducting Metal-Oxides and GHz-THz Photoconductivity as a Performance Metric: Nicholas Hight-Huf, UCSB

06/11/09:

Confinement Matters: Quantum Posts for Terahertz Emitters: Gernot Fasching, UCSB

Awards Administered

(July 2008 – June 2009)

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

Guenter Ahlers

National Science Foundation, DMR-0702111

Turbulent Convection in a Fluid Heater from Below

05/01/07-04/30/10 (04/30/12)

\$465,000 (\$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.

S. James Allen

Kevin Plaxco

ARMY, W9119NF-06-1-0241

**Terahertz/Optical Two Color Non-Linear Sensing of Liquid Biochemical Agents
(II.B.1.e)**

06/15/06-06/30/09

\$484,216

The species-specific sensor of biochemical agents in water is based on terahertz/optical sum and difference frequency generation that appears only in chiral liquids. Terahertz sidebands on an optical probe, at the sum or difference frequency, are allowed in a liquid only in the presence of chiral symmetry and are free of signals from non-biological material. The process is doubly resonant – the terahertz radiation resonantly drives the macromolecular vibrations while the optical probe resonates with an electronic transition in a chromophore. At the same time the appearance of a sideband requires a spatial overlap of the driven macromolecular vibration and the chromophore. The terahertz frequency dependent appearance of the sideband on the optical probe signals the presence of the biomaterial of interest. While chiral allowed sum and difference frequency generation has been documented in the near-IR/optical, the phenomenon has not been exploited in the terahertz part of the spectrum. Spectrometer development uses the UCSB terahertz free-electron lasers to explore and develop this phenomenon in this part of the spectrum. The terahertz sideband spectrometer as biochemical sensor uses terahertz harmonic generators in conjunction with narrow line width semiconductor diode lasers.

S. James Allen

Sandia National Laboratories, 622559

Terahertz Resonant Plasmonic Detectors

07/01/06-09/30/07

\$40,000

This contract addresses the research and development of 2-D plasmon-based resonant, tunable, terahertz detectors. The PI shall evaluate their potential for terahertz spectroscopy on a chip, terahertz focal plane arrays and terahertz focal plane arrays for spectroscopic imaging.

S. James Allen
Sandia National Laboratories, 784231
Terahertz Resonant Plasmonic Detectors
03/06/08-09/30/08
\$40,000

The objective is to test, model and document plasmonic resonant detectors with integrated and voltage controlled barrier rectifiers fabricated at Sandia.

Bjorn Birnir
Marine Research Institute (Iceland) SB080063
Simulations of Complex Schools of Fish
11/01/07-10/31/09
\$64,548

This is an agreement to conduct research and simulations on capelin migration in Icelandic and adjacent waters, based on data collected and provided by the Marine Research Institute with the aim to further understanding underlying dynamics of changes in the migration pattern of capelin in these waters.

Jeffrey Bode
Camille & Henry Dreyfus Foundation, SB#040029
Design, Synthesis and Applications of Adaptive Organic Molecules
10/01/03-09/30/08
\$40,000

This award supports the design and synthesis of a new class of organic molecules that can spontaneously adjust their shape and properties to adapt to their environment. Potential applications of these materials include drug discovery, chemical sensing, and drug delivery. We have completed the chemical synthesis of a functionalized core and demonstrated the dynamic nature of these model compounds. This represents the first rational synthesis of a designed, adaptive organic molecule. Currently we are developing technologies for the specific modification of the dynamic core to prepare molecules with wide-ranging applications and to utilizing these unique structures for fundamental chemical studies.

Jeffrey Bode

National Science Foundation, CHE-0449587

CAREER: Development and Applications of Catalytic Generated Activated Carboxylates

01/15/05-12/31/10

\$583,280

Intramolecular redox reactions of α -functionalized aldehydes mediated by N-heterocyclic carbenes (or heterocyclic ylides) lead to the catalytic generation of activated carboxylates, suitable for the synthesis of esters, amides, and other carboxylic acid derivatives under economical and environmentally friendly reaction conditions. The discovery of this novel reactivity, mediated by an organic catalyst, of α -heteroatomic and α,β -unsaturated aldehydes opens a broad range of mechanistically unique pathways for the synthesis of chiral carboxylic acid derivatives, including anti- β -hydroxyesters and β -amino peptides. The design and application of chiral heterocyclic salts for catalyzing this novel process will provide an enantioselective method for directly controlling the absolute stereochemistry concomitant with esterifications and peptide couplings, and has the potential to supplant traditional multi-step chiral auxiliary based methodologies. By developing means of effecting the direct, enantioselective synthesis of amides from α,β -didehydroamino aldehydes, a waste-free, atom-economical approach to the synthesis of poly- α -amino-peptides from achiral precursors will emerge. The unique reactivities of unsaturated aldehydes under these catalytic conditions will enable novel carbon-carbon bond forming processes, including new annulation reactions affording lactones, lactams, and cyclopentanones, thereby providing a long-sought method for the direct, intermolecular synthesis of hetero- and carbocycles from stable, readily available starting materials. Applications of these new reactions include the synthesis of (1) short, biologically active α - and β -peptides, (2) the kalafungin class of naturally occurring antibiotics, and (3) the antibiotic moiramide B, which is active against drug resistant bacterial strains. With the support of this CAREER award from the Organic and Macromolecular Chemistry Program, Professor Jeffrey W. Bode, of the Department of Chemistry and Biochemistry at the University of California, Santa Barbara, is developing new reactions catalyzed by simple organic molecules rather than by metals. This reaction chemistry not only offers promise of great chemical selectivity, but also represents an economical, environmentally friendly ("green") approach to organic synthesis, eliminating the use of potentially hazardous metals and greatly reducing waste generation. Professor Bode will exploit the newly discovered reaction chemistry for the synthesis of a variety of products, including biologically active polypeptides and antibiotics, demonstrating the potentially broad applicability of this chemistry in the synthesis of important products. He will also engage undergraduate students, both at UCSB and from local community colleges, in an alternative sophomore level organic laboratory course aimed at exposing them to hands-on training in the realities of inquiry and research based organic chemistry.

Jeffrey Bode
Research Corporation, CS1392
New Ligation Reactions for the Synthesis of Biomolecules and Biomaterials
07/01/06-06/30/11
\$100,000

The next generation of therapeutics, functional materials, and designed nanostructures are inaccessible with existing methods of molecular synthesis. To address this, we are developing new organic reactions that enable both stepwise and fragment condensation approaches to large, functionalized structures under aqueous conditions and without reagents, catalysts, or by-products. These processes, and others under development in our laboratories, will provide the foundation for a new approach to the synthesis of complex molecules including glycopeptides, tailored biomaterials, and nanoscale assemblies. As a specific example, we detail new approaches to the synthesis of poly- α -peptides by a novel ligation reaction that forms amide bonds under aqueous conditions, without reagents, and produces only carbon dioxide as a by-product.

Jeffrey Bode
NIH Center for Scientific Review, R01 GM076320
New Reactions for Direct, Native Peptide Ligations
09/01/06-08/31/08
\$221,553
Supplement for graduate student, Melissa Flores
09/01/06-08/31/08
\$31,801

The goal of the proposed research is to develop a comprehensive method for the direct coupling of unprotected molecules via a new chemoselective amidation reaction. The basis for this project is the reagent-less reaction of α -ketoacids and *N*-alkylhydroxylamines to give amides via decarboxylation and dehydration. These studies will provide new methods for the synthesis of biomolecule targets including proteins, glycopeptides, and peptidomimetics. The proposed research will provide a new chemical tool for the direct synthesis of amides under physiologically compatible reaction conditions. It will significantly impact the synthesis of complex biomolecules including proteins, glycoproteins, peptidomimetics, and biocompatible materials.

Jeffrey Bode

Nancy Carrillo

NIH, National Institute of Neurological Disorders & Stroke, F31 GM078854

Ruth L. Kirschstein Pre-Doctoral Fellowship: Aqueous Synthesis of Poly-Beta-Peptides

09/01/06-08/31/08

\$26,779

The discovery that oligomers of beta-amino acids adopt stable secondary structures has sparked immense interest in the synthesis, study and application of this peptidomimetics. However, some of the drawbacks on the preparation of poly-beta-peptides include the use of large molar excesses of expensive coupling reagents and multiple steps. Based on the recently developed ketoacid-hydroxyamine peptide ligation discovered by the laboratories of Dr. Jeffrey Bode, we have synthesized poly-beta-peptides by iterative, reagentless coupling of isoxazolidine monomers under aqueous conditions. Our long term plan is to synthesize using our methodology, other classes of isoxazolidine monomers including cyclic-beta-peptides which have shown to be potentially useful as therapeutic agents for the management of biomedical problems. Furthermore, we hope to perform solid phase synthesis of poly-beta-peptides using our current solution phase methodology. In addition, we plan to use our isoxasolidine approach to beta-peptide synthesis to prepare the beta-peptide analogue of the HIV Tat DNA binding protein and examine its attachment to nucleic acids or drug candidates.

Dirk Bouwmeester

Lawrence Coldren

Pierre Petroff

National Science Foundation, PHY-0304678

NIRT: Quantum State Transfer Between Photons and Nanostructures

08/15/03-07/31/08

\$1,620,910

Photons have proven to be most useful for encoding special quantum states and for transmitting them through free space or optical fibers. For local quantum-state operations photons are less favorable and well-localized quantum systems are desirable. In this respect quantum dots, often referred to as artificial atoms, are particularly attractive. This research aims at combining the advantages of photons with those of artificial atoms. The main objective is to transfer the polarization quantum state of a single photon onto excitons in quantum dots and visa versa. The anticipated results are: a novel positioning technique for a quantum dot in the center of an optical waveguide, the demonstration of a single-photon absorption and reemission by a single quantum dot inside a micro-pillar with intrinsic lensing, the demonstration of the polarization quantum-state transfer between single photons and single quantum dots, and creating entanglement between a quantum dot and a photon and between two quantum dots. The first requirement to achieve the objectives is that the coupling between photons and quantum dots has to be

resonant in order to preserve the quantum-phase coherences. For this optical-cavities resonant both with the incoming photon and the quantum dot inside the cavity will be used. Two novel ways of achieving a strong optical mode overlap with the quantum dots will be explored. The first is to use quantum dots inside micro pillars that containing optical lensing through the use of tapered oxidation layer. The second is to develop a technique to position a single quantum dot in the center of an optical micro cavity. The second requirement is that the quantum dots have to be effectively symmetric in order to obtain exciton spin degeneracy. For this magnetic fields and/or strain-induced effects on the micro-pillars will be explored. The third requirement is that the reemitted photon from the quantum dot should be distinguishable from photons reflected from the sample surface. For this a Michelson interferometer will be used where the two end mirrors are replaced by one micro-cavity containing a quantum dot on resonance and one micro-pillar containing no quantum dots on resonance. Reaching the objectives will be a major step forwards in quantum-state control and harnessing and understanding quantum decoherence in nano-structures. The research is based on a close collaboration between the Materials, Engineering and Physics Departments at the University of California Santa Barbara. This collaboration provides an excellent opportunity for young researchers to perform interdisciplinary research on important topics in quantum (and classical) communication and information processing and in nano-structure fabrication. Reaching the objectives will initiate future research in storage of quantum information and in implementing the quantum repeater scheme (enabling long-distance quantum cryptography), quantum error correction and quantum networks.

Dirk Bouwmeester

Deborah Fygenon

National Science Foundation, PHY-0504825

Quantum Superposition States of a Mirror

08/01/05-07/31/08

\$360,000

Quantum Mechanics is based on a wave-mechanical description of a system and on the von Neumann postulate (1920s) that a quantum measurement results in an indeterministic outcome. The wave-mechanical description allows for superposition states of a system (e.g. an object being in two places at the same time), and the von Neumann postulate implies that one cannot directly detect such a superposition. Models of environmental induced decoherence do give an explanation of why quantum superpositions are not observed in everyday life, however the indeterministic nature of the measurement outcome is still the topic of many debates. The aim of this research proposal is to create a quantum superposition states involving of order 10^{14} atoms. Such quantum superposition states will be ten orders of magnitude more massive than any quantum superposition observed to date and will therefore provide a fundamental test of quantum mechanics in a new regime. The experiment contains a tiny mirror (smaller in diameter than the thickness of a human hair) that is part of an optical cavity, which forms one arm of an interferometer. The mirror is mounted on a tiny Silicon rod and can be displaced by the multiple reflections of a photon. A single photon is sent into the interferometer and will evolve into a superposition of being inside the optical cavity with the tiny mirror, thereby slightly displacing it, and being in the other arm of the interferometer, leaving the mirror at rest. The superposition of a single

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

photon is therefore transferred to a superposition of the mirror, or more precise, the mirror becomes entangled with the photon. By observing the interference of the photon leaving the interferometer one can study the creation and decoherence of superpositions involving the mirror. Preliminary experiments have been supported by a one-year NSF exploratory-research grant and led to remarkable initial progress; a high-quality Bragg mirror of diameter 20 microns has been fabricated using a focussed ion beam and has been positioned onto a Silicon cantilever [tip of an atomic force microscope (AFM)]. The cantilever/mirror system has been piezo-positioned to be the end mirror of an optical cavity. Measurements in air showed an initial cavity finesse of 1000. The individual components of the precision measurement system will be of interest for applications in many other fields with direct benefits to society. Anticipated spin-off projects are ultra-fast switchable mirrors (for optical communication), ultra-high resolution AFM readout, and optical cooling of micro-mechanical oscillators (for position measurements). The project will provide excellent training since it combines fundamental research interests with cutting-edge technologies. Since the project involves different subprojects, it is the intention to have several undergraduate researchers assisting the project each summer, as well a high-school students participating in the UCSB summer science education program.

Dirk Bouwmeester

National Science Foundation, PHY-0804177

Quantum States of OptoMechanical Structures

08/01/08-07/31/09 (07/31/11)

\$280,000 (\$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 multi-disciplinary and international environment.

Michael Bowers

University of Warwick, HR/DD/13 12763

Toward an Antemortem Test for Bovine Spongiform Encephalopathy: An Ion Mobility/Mass Spectrometry Approach

01/01/05-06/30/09

\$485,469

The need for an antemortem test for TSE diseases is apparent and urgent, but the difficulties are formidable. Small fractions of PrP^{Sc} must be detected in the presence of large excess of native PrP^c in accessible body fluids that contain only minute amounts of total PrP. Since PrP^{Sc} and PrP^c have the same primary structure any method must detect differences only in folding (shape) using methods that do not induce isomerization between the isoforms. In this proposal the ultra sensitive techniques of Ion Mobility Spectrometry and Mass Spectrometry (IMS/MS) will be combined and provide unambiguous differentiation of the isoforms.

Michael Bowers

National Science Foundation, CHE-0503728

Conformation, Hydration, Metal Ion Interactions and Aggregation States of Peptides, Proteins and Oligonucleotides

07/01/05-04/30/09

\$632,877

This research is supported by the Experimental Physical Chemistry Program to examine molecules and systems of biological importance, using mass spectrometric methods. Work will focus on the following specific areas: (1) duplex formation in oligonucleotides, (2) solvation energies, entropies, and diagnostics, and (3) structure and energetics of metal ion binding to nucleotides, peptides, and proteins. Ion-mobility-based mass spectrometry will be used for structural (cross-section) measurements and ion-neutral equilibrium methods for hydration studies. High-level electronic structure calculations and/or molecular dynamics calculations will accompany experiment in all cases. This project presents the opportunity to make significant inroads toward developing new ways to solve biological problems using mass spectrometry. For example, outcomes could help unravel fundamental and practical issues such as water molecule binding to biomolecules. Students and postdoctoral associates will have valuable

research education opportunities in both experiments and theory, and they will participate in designing new forefront technical methodologies.

Michael Bowers

Air Force, FA9550-06-1-0069

POSS and Metal Clusters: Structures and Energetics

01/01/06-11/30/09 (11/30/10)

\$747,000 (\$936,000)

There are several objectives for this proposal:

1. Structure and Characterization of Polyhedral Oligomeric Silsesquioxane (POSS) attached to Polymer Backbones: The POSS family of molecules has recently generated great interest due to their inherent thermal and chemical stability and their ability to improve the thermal, physical and chemical properties of host polymer systems. We have developed ion-mobility-based mass spectrometric methods suitable for characterizing a wide variety of POSS cages. In the coming three years, these methods, coupled with extensive molecular modeling will be applied to POSS cages covalently bound to oligomers of a variety of organic polymers. We will collaborate with a number of synthetic research groups in the development of rational synthetic strategies to produce these materials.

2. Size-Selected Structures and Ligand Binding Energies of Metal Clusters: In recent years there has been a major renaissance in the study of small metal clusters as catalytic agents for select, important industrial processes. Of special importance are the clusters of coinage metals: gold, silver and (possibly) copper. At UCSB we have constructed a unique instrument for the deposition and characterization of size-selected coinage metal clusters on metal oxide surfaces, funded by a multi-investigator DURINT grant. There are several aspects of this work that are strongly complemented by gas phase studies, Careful STM measurements have established that clusters of four or more gold atoms have specific structures on the surface and that the onset of the transition from 2-dimensional to 3-dimensional surface clusters occurs below $n=8$. It will be very important to know the actual structures of the species that are deposited at low energies onto the surfaces to see if they correlate with observed surface structures. Theory also plays a large role in interpreting the structure and reactivity of surface-deposited systems. Careful measurement of structures and ligand binding energies of size- and charge-selected gas-phase clusters is crucial for providing experimental benchmarks for testing theoretical models. Finally, shape and ligand binding energy studies over large cluster size ranges allows direct observation of atomic to bulk transitions, an area where much is speculated but little is known.

Michael Bowers
UC Los Angeles, SB070075
Pathogenic Protein Folding and Human Disease
09/01/06-07/31/09 (07/31/11)
\$775,519 (\$1,305,939)

The objective of this research is to understand, on a molecular level, the folding and assembly of A β -protein alloforms. Recent results indicate small, soluble oligomers of A β are responsible for initiating a pathological cascade resulting in Alzheimer's disease (AD). A β 42 has been shown to be the primary neurotoxic agent even though A β 40 is nearly 10 times more abundant. Single-point amino-acid substitutions at positions 22 and 23 in A β 42 account for a variety of familial forms of AD. It is our hypothesis that A β 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 A β 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 β monomers and to determine how these structures change with single-amino-acid substitution, oxidation or other simple sequence modification, (2) to structurally characterize A β 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 of A β and modified forms of A β 40 and A β 42.

Steven Buratto
Michael Bowers
Department of Energy/Miscellaneous Offices and Programs, DE-FG02-06ER15835
Chemical Imaging with 100nm Spatial Resolution
09/01/06-08/31/09
\$596,299

Over the past decade high resolution optical microscopy methods have been utilized with great success to image the absorbance, luminescence, photoconductivity and Raman scattering of thin films and surfaces with spatial resolution of the order of 100nm. Using conventional far-field optics (i.e. microscope objectives), laser scanning confocal microscopy (LSCM) is capable of probing materials with spatial resolution approaching 200 nm and single molecule sensitivity in fluorescence and surface-enhanced Raman contrast. In addition, a new scanned probe microscopy, near-field scanning optical microscopy (NSOM) method has been developed with the same capabilities and array of applications as

LSCM but with spatial resolution enhanced by nearly an order-of-magnitude. Despite such wide applicability, these imaging methods still lack chemical specificity and often produce images where it is difficult to determine the chemical origin of the image contrast. In order to address this deficiency we propose to combine, in a single instrument, the high spatial resolution microscopy techniques of LCSM and NSOM with the chemical specificity and conformational selectivity of ion mobility mass spectrometry. We will adapt the source chamber of an ion mobility apparatus to include a combination scanning confocal/near-field microscope. The optical microscopy will be performed in vacuum and an image with luminescence, transmission (absorption) or Raman contrast will be recorded using either the microscope objective or the NSOM optics. In order to determine the chemical contrast from selected domains in the optical image, we will position the sample to the desired spot with the scanning electronics and vaporize molecules from the selected region via laser desorption ionization using the imaging optics. A mass spectrum and/or an arrival time distribution (ATD) will then be recorded from the gas-phase molecules. This data will provide a chemical signature (i.e. mass measurement) and a shape distribution for a given species (ATD) within the localized region of the sample.

Steven Buratto

Michael Bowers

Horia Metiu

National Science Foundation, CHE-0749489

Model Nanocluster Catalysts: The Role of Size, Shape and Composition on the Catalytic Activity on Monometallic, Bimetallic and Metal Oxide Clusters on Oxide Surfaces

04/01/08-03/31/10 (03/31/11)

\$369,000 (\$536,000)

In this research supported by the Analytical and Surface Chemistry Program, Professors Buratto, Bowers, and Metiu and their groups will prepare, characterize, and test three new types of nanoscale catalysts, having one feature in common: very small, isolated, well-defined, catalytically active sites. They will prepare and study (a) very small Au_n and Ag_n mass-selected clusters supported on oxide, (b) very small mass-selected, binary clusters such as Pd_mAu_n supported on oxides, and (c) very small, mass-selected oxide clusters supported on oxides. A variety of techniques will be used, in a concerted manner, to study these important catalytic processes: model catalytic systems will be prepared by depositing mass-selected clusters on oxide surfaces to ensure atom-by-atom control of catalyst size; all samples will be prepared and studied in ultra-high vacuum by surface science techniques (AES, XPS) as well as by STM/ AFM before, during and after the catalytic chemistry; and density functional theory (DFT) will be used to calculate the structure of the clusters, their XPS spectrum and their chemical activity. Through the work proposed here they will develop a detailed understanding of the catalytic chemistry of these materials and find out how this chemistry depends on size, composition and the nature of the substrate. While the focus of the research is on the catalytic activity of specific nanoscale catalysts, there is a high probability that the results will be applicable to other systems. In addition, it is

hoped that the concepts developed through this research will help optimize important industrial processes using these nanoscale catalysts and provide insight into the discovery of new nanoscale catalytic materials. The research funded by this grant will be interdisciplinary. Graduate students will interact continuously with three different research groups, will have daily contact with other outstanding scientists, and will acquire hands-on experience in a large number of techniques of surface science, gas-phase chemistry, scanned probe microscopy, and high level theory. The research will provide a valuable opportunity for graduate education, found in very few places in the world. Researchers supported by this grant (including PIs) will also be active in outreach to K-12 schools in the Santa Barbara area to present a tutorial on an atomistic view of heterogeneous catalysis and to show an atomically-resolved picture of our model catalyst systems. This will be included in the currently active outreach program in the chemistry department at UCSB. A series of lectures on catalysis by nanostructures will be developed and included as part of a course in nanoscience currently taught in the materials chemistry curriculum.

David Cannell

National Aeronautics and Space Administration, NNCO4GA45G

Gradient Driven Fluctuations

12/04/03-11/30/08

\$471,000

We will work with our collaborators at the University of Milan (Professor Marzio Giglio and his group-supported by ASI) to define the science required to measure gradient driven fluctuations in the microgravity environment. Such a study would provide an accurate test of the extent to which the theory of fluctuating hydrodynamics can be used to predict the properties of fluids maintained in a stressed, non-equilibrium state. As mentioned above, the results should also provide direct visual insight into the behavior of a variety of fluid systems containing gradients or interfaces, when placed in the microgravity environment.

During the past year, we have used the UCSB prototype to demonstrate that the overall design is functional. In doing this we have obtained data for the fluctuations in a single-component fluid heated from above, extending to wavelengths that have not been accessible in the past. The companies responsible for constructing flight hardware have been placed under contract by the European Space Agency. We met with them once shortly after they were selected, and again in early August for what ESA calls the "Preliminary Design Review". PDR went well, and both ESA and the science teams (UCSB and U. of Milano) are relatively confident that the companies will be able to perform.

David Cannell
National Aeronautics and Space Administration, NNX08AE53G
Gradient Driven Fluctuations
03/01/08-02/28/10
\$125,000

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 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.

Andrew Cleland
National Science Foundation, DMR-0605818
Mechanical Quantum Resonators: Quantum Optics with Phonons
07/01/06-06/30/10
\$355,000

Quantum mechanics controls the behavior of very small, atomic-scale systems like the hydrogen atom and the electron. Demonstrations of the applicability of quantum mechanics to larger scale systems, especially ones with millions or more independent atoms, are challenging due to the need to isolate the system of interest from the environment that surrounds them, an environment that demolishes the quantum effects so peculiar to our classical experience. To date, no clear demonstration of quantum effects in large systems has been performed, certainly not in large mechanical systems. This project will focus on the construction of small mechanical resonators, similar to quartz crystals used to time computer circuits, sufficiently disconnected from the rest of the world to allow quantum effects to be displayed in an unambiguous fashion. In particular, the quantum nature of vibrational energy, which is predicted to change in steps rather than in a continuous fashion, will be explored in detail. The multidisciplinary project integrates research and education in order to train students and postdoctoral researchers in modern methods required to address this key problem in physics, which will be integrated with engineering and nanotechnology to achieve the goals set forward here. The acquired interdisciplinary skills, which include state-of-the-art nanofabrication and radiofrequency and microwave technology, prepare the trainees for careers in academe, national laboratories, and industry.

Frederick Dahlquist
Public Health Service/National Institutes for Health, RO1 GM059544
Mechanistic Studies of Bacterial Chemotaxis
03/01/04-07/31/09
\$1,385,070

The original goal of this research was to define the molecular mechanisms that underlie bacterial chemotaxis. It has become clear that bacterial chemotaxis employs “two component” regulation in its basic biochemistry. This mechanism is common to many bacterial signaling pathways (at least 30 *in Escherichia coli*). These feature a specific histidine auto-kinase that phosphorylates a specific response regulator domain on an aspartate residue that is conserved in the family of response regulators. The phosphorylation event modulates the interaction of the response regulator domain, resulting in enhanced or diminished interactions with other domains or proteins. Thus our long-term has expanded to include a more general understanding of the consequences of phosphorylation of response regulator domains while we continue our focus on bacterial chemotaxis.

Frederick Dahlquist
Public Health Service/National Institutes for Health, R01 GM057766
Protein Energy Landscapes by NMR and Single Molecules
03/01/04-07/31/08
\$641,597

This research is concerned with probing the energy landscape in order to define its shape both near the true minimum and far from it. We previously developed a new nuclear magnetic resonance approach, based on relaxation dispersion measurements. This will allow us to gain access to new information about the energetics and structural location of higher energy conformations whose equilibrium populations may be present in only a few percent of the dominant conformation(s). In addition, we have used single molecule, mechanical unfolding experiments to probe the landscape more widely.

Frederick Dahlquist
Bradley Chmelka
Patrick Daughtery
Songi Han
Luc Jaegar
John Lew
David Low
John Perona
Kevin Plaxco
Norbert Reich
Public Health Service/National Institutes for Health, S10 RR019899
Purchase of an 800 MHz NMR Spectrometer
08/01/06-07/31/09
\$2,000,000

Purchase of an 800 MHz NMR Spectrometer.

Deborah Fygenon
Dirk Bouwmeester
National Science Foundation, CCF-062257
DNA Patterned Pairs of Colloidal Quantum Dots: A Scalable Approach to Computing Without Wires
09/01/06-08/31/09
\$300,000

To reduce the size of computer architecture and test a revolutionary new approach to computation, we will investigate fully self-assembled arrays of classical and quantum bits that are addressed by optical signals only. As bits we propose to use single electron spins in colloidal quantum dots (cqdots). Every cqdot has a specific resonance frequency at which the absorption of a photon can lead to the formation of a trion state (two electrons and one hole confined within a quantum dot). Trion states have large electric dipole moments and can therefore interact over distances of the order of 10 nm. We will leverage the polarization of the illuminating light and the Pauli exclusion principle to control trion formation and subsequently detect the spectral effect of dipole-dipole interactions between cqdots spaced 5 to 10 nm apart. In this manner, we have as a long-term goal the physical realization of theoretical schemes for quantum computing. On the way to this goal, we will explore simplified approaches that are also very interesting from the perspective of classical computation and data storage. For the three-year period of the proposed research, our primary contribution to the quest for all-optical classical and quantum computation will be to address the challenge of nanometer positioning of

colloidal quantum dots and to study their optical interactions. Our approach will be to combine self-assembled DNA scaffolds with site-specific binding elements to produce an array of optically active colloidal quantum dots. Self-assembled DNA scaffolds leverage the intrinsic specificity of Watson-Crick base-pairing to organize millions of atoms into close-packed arrays of the familiar double-helical structure with nanoscopic precision. Modern synthesis methods allow decoration of specific atoms in the DNA structure with chemically reactive groups. These reactive groups can be chosen to form covalent links to molecules that stabilize the surface of colloidal quantum dots. By placing the reactive groups at specific sites on the DNA scaffold, pairs of dots and linear or two-dimensional arrays of dots will be patterned, with a spacing that favors quantum mechanical interactions between dots. The resulting structures will be characterized by scanning probe microscopy and the interactions probed by optical pump-probe measurements.

The research will be carried out by a cross-disciplinary research team at the University of California Santa Barbara that is anchored by expertise in self assembly of DNA, the synthesis of colloidal quantum dots and their attachment to functionalized elements at specific locations (Fygenson), and expertise in quantum-optics and solid-state experiments analyzing coupled quantum dots embedded in bulk semiconductor material (Bouwmeester). We will collaborate strongly with Paul W. K. Rothmund, in the Department of Computer Science at Caltech, who recently invented an powerful new class of self-assembling DNA scaffolds that can template arbitrary complex patterns with 6 nm resolution.

Songi Han

Frederick Dahlquist

Mark Sherwin

Louis-Claude Brunel

Johan van Tol

National Science Foundation CHE-0821589

MRI: Development of a 240 Hhz Pulsed Electron Paramagnetic Spectrometer with Nanosecond Time Resolution

10/01/08-07/31/11

\$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

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

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

Public Health Service, National Institutes of Health, R01 GM040287

Metal-Mediated Routs to Biaryls

04/01/04-03/31/09

\$1,227,821

Biaryls represent a major area of natural and unnatural products chemistry. Given the widespread occurrence of physiologically active compounds in nature that contain a biaryl axis, many of which due to hindered rotation possess an element of axial chirality, methodology is needed to respond to these special synthetic challenges. Representative targets which highlight existing limitations yet which provide opportunities for significant advances in this area include the clinically essential antibiotic vancomycin, and the potent *anti*-AIDS biaryls, the michellamines. Using a judiciously placed internal phosphine ligand in an aryl halide coupling partner, the directionality associated with our key Suzuki-biaryl coupling-based approach to the vancomycin biaryl and the subunits of the michellamines will be controlled. Alternatively, a conceptually new entry to stereocontrolled biaryls, as applied to vancomycin, will be pursued using a Bergman cyclization of a substituted nonracemic endiyne.

The chemistry of biaryl constructions, which is usually effected in solution using Pd(0) catalysis, is to be pursued *via* an alternative metal system: nickel. Proposed herein are new methods for heterogeneous catalysis based on Ni/C, to be examined under microwave conditions, and the next generation species nickel-on-graphite (“Ni/C_g”), which appears to offer a different reactivity profile.

Finally, a new series of nonracemic ligands based on the binaphthyl core, in particular of NOBIN, will be constructed. The approach presented will provide entry to unprecedented substitution patterns on this ligand system, as well as opportunities for their mounting on a solid support for use, and re-use, under heterogeneous conditions. A particular, albeit representative, application of a novel substituted *cyclo*-NOBIN will be studied for selected asymmetric aldol reactions.

Bruce Lipshutz
National Science Foundation, CHE-0550232
Asymmetric Catalysis with Ligated Copper Hydride
02/01/06-01/31/10
\$592,000

This project is focused on the theme of catalysis, specifically involving copper(I) hydrido complexes that are mainly ligated by nonracemic bis-phosphines ((L*)CuH). The action of catalytic (L*)CuH on aryl ketone intermediates will form products useful for the synthesis of known pharmaceuticals. Catalytic (L*)CuH will be used in new contexts that will afford valued nonracemic intermediates for synthesis, extending the limits of this CuH chemistry. A newly designed ligand will be synthesized to test the factors that may control both reaction rates and enantioselectivities. Experiments aimed at investigating the nature of the species (L*)CuH are planned, supporting the goal of providing a practical source of (L*)CuH; i.e., effectively CuH in a Bottle. Using boranes as the stoichiometric source of hydride, new inroads to boron enolates will be developed and used to synthetic advantage based on transmetalations. Finally, copper-in-charcoal (Cu/C) will be explored as a potential new approach to asymmetric (heterogeneous) organocopper chemistry. Catalysis represents a powerful tool in the development of more economical and environmentally friendly technologies. Professor Lipshutz and his students are exploring new ways to catalyze organic chemical transformations using copper compounds. These copper compounds are significantly less expensive than the more commonly used precious metal catalysts and offer unique chemical reactivity as well. By developing these new catalysts, Professor Lipshutz is developing methodologies that may be generally and broadly applicable in the synthesis of complex organic molecules and pharmaceuticals.

Bruce Lipshutz
UCSB
The Green Initiative Fund (TGIF)
Getting Organic Solvents Out of Organic Reactions
06/01/09-06/30/10
\$22,500 (\$45,000)

Our plan is to devise up to three new experiments that will teach high school and college level students about green chemistry. These will focus on eliminating the major source (i.e. 75+%) of chemical waste: organic solvents. The nanotechnology ("micellar catalysis") in hand and upon which these new experiments are to be based will allow for them to be run in water (actually seawater!) at room temperature; no additional energy consumption/cost should be needed. If realized as envisioned, lab hoods may not even be required. This pilot study may, therefore, be a model that further encourages those who oversee teaching labs in Chemistry to design elements of sustainability (i.e. "benign by design") into their curricula so as to focus on minimizing use of organic solvents.

R. Daniel Little

American Chemical Society, PRF#43443-AC1

Catalytic, and Potentially Enantioselective ERC and EHC Reactions

07/01/05-08/31/08

\$80,000

In this award we describe the use of nickel (II) salen as a catalyst/mediator in the ERC and EHC reactions. To the best of our knowledge, the ability to affect either reaction in this manner is a first of its kind. Preliminary evidence is provided to suggest that the first electron transfer occurs *via* a ligand-centered process. It is upon this topic/process that we will focus our attention. Through additional detailed investigations involving voltammetric inquiries, semi-empirical quantum calculations, and ESR probes, as well as through structural variations of the substrate, the metal, and the ligand, we intend to optimize the chemistry, expand the scope of the transformations, and gain additional levels of understanding mechanistically. We hope to be able to perform the reactions enantioselectively, and plan to use what we learn to synthesize cinnamolide, a simple, yet interesting natural product that is effective in halting bleeding.

R. Daniel Little

Robert Jacobs

Army, W81XWH-06-1-0089

The Role of the Pseudopterosins and their Analogs in Wound Healing

11/20/06-10/19/09

\$991,582

Severe injury from chemical or physical sources continues to be a serious and challenging medical problem from the perspective of successful treatment, survival, and recovery. A physical surface injury to the skin of most animals initiates a complex series of immune and physiological responses involving pain, inflammation, wound repair and scar formation. The total process of wound repair or wound healing is not homogenous among species but many components of the response are phylogenetically conserved and are observed in very primitive unicellular algae and ciliates.

In vertebrates including man certain forms of injury are followed by a major initial infiltration and concentration of neutrophils at the sight of injury. During the early stages of phagocytosis, these cells degranulate and release stored enzymes such as myeloperoxidase, proteases, lipases, and pro-inflammatory eicosanoids and chemotactic factors that attract additional immune cells. They also produce reactive oxygen species, alter vascular permeability, and induce swelling. Most cells also contribute to this early stage by releasing histamine and other autocooids.

We hypothesize that donor sites in patients undergoing repeated reconstructive surgery may represent a clinical condition that can be simulated experimentally by topical treatment of mouse ears with the irritant phorbol myristate acetate (PMA). We base our hypothesis on the fact that Pseudopterosin A and

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its analogs block infiltration of neutrophils in the PMA treated mouse ear and also block phagocytosis and degranulation in cell culture models. Recent phase 2 clinical trials have shown that topical application of pseudopterosin A methyl ether significantly increased healing rate of donor sites in burn patients. We believe this may be in part the result of diminished pro-inflammatory mediators at the wound site. We wish to exploit these results and propose to optimize the potency and efficacy of the pseudopterosin pharmacophore, increase its bioavailability and provide a new molecule that can be readily synthesized.

Philip Lubin

Jet Propulsion Laboratory, JPL1289807

Planck Educational and Public Outreach Effort at UCSB

09/21/06-09/30/08

\$103,500

The theoretical framework in community ethnography, and modern physics education research, and theories of intelligence and creativity, has already been established as part of the process of advancement to candidacy for a Ph.D. in Physics Education (van der Veen-Davis, June, 2006). During the 2006-07 academic year, we will use funds for the support of this work, leading to the development and testing of the symmetry-based curricular materials with undergraduates and pre-service science teacher candidates at UCSB. Using the Planck mission as a paradigm of studying symmetry and deviations from symmetry in the universe will be used throughout as appropriate. This research will be undertaken in three phases initially: 1): Interviews with students and teachers, both personal and through surveys, questionnaires and classroom observations. 2): Curriculum development and 3): Curriculum testing and evaluation.

Philip Lubin

Jet Propulsion Laboratory, JPL1367008

Planck Educational and Public Outreach Effort at UCSB

02/10/09-09/30/13

\$20,000 (\$62,000)

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.

Philip Lubin
Jet Propulsion Laboratory, JPL1372889
W-Band Amplifier Assemblies
04/06/09-05/30/09
\$12,000

UCSB will provide 40 W Band amplifier bodies to JPL based on the drawing JPL provided. UCSB has experience in making these mm wave amplifier bodies and knows what is needed. UCSB expects to provide the first batch in approximately 30 days followed by the remainder within 60 days after acceptance of the proposal.

Douglas Scalapino
Oak Ridge National Laboratory, 4000068439
Exploration of Routes to Higher Superconduction Transition Temperatures
04/14/08-09/30/10
\$210,666

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
Pierre Petroff
Craig Pryor
Jelena Vuckovic
National Science Foundation, CCF-0507295
NIRT: Semiconductor Nanostructures and Photonic Crystal Microcavities for Quantum Information Processing at Terahertz Frequencies
08/01/05-07/31/09
\$1,500,000

This grant will explore the fundamental physics of elements in a proposed semiconducting quantum information processor (QIP) which is potentially scalable to ~1000 quantum bits (qubits). The qubits in the envisioned QIP are the two lowest orbital states of electrons bound to shallow donors (D0) in GaAs or bound in elongated self-assembled quantum dots called quantum dashes (QDAs). QDAs will be grown by molecular beam epitaxy on patterned substrates. The resonance frequency of D0 and QDA-

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

based qubits will be between 1 and 4 Terahertz (THz). The energy relaxation and decoherence rates of these qubits will be measured, and are predicted to be slow because the resonant frequencies are well below that of an optical phonon. GaAs and Si Photonic crystal resonators for THz frequencies will also be fabricated and characterized. Finally, qubits will be incorporated into resonators and reversible coupling of energy between the resonator and qubits will be investigated. This research program works at two scientific and technological frontiers: harnessing quantum mechanics for information processing, and developing the portion of the electromagnetic spectrum between 1 and 10 THz (THz-1 THz=one trillion cycles/s). The research will explore a new approach to quantum information processing in semiconductors, enhance our fundamental understanding of the transfer of information and energy between simple quantum systems and their semiconducting hosts, and create new materials and structures in which to store THz light and control its interaction with matter.

Mark Sherwin

Florida State University, R00501

Instrumentation for Materials Research, Major Instrumentation Project: Free-Electron Laser Facility for Spectroscopy in the Terahertz to Near-Infrared Range Under Very High Magnetic Fields

11/01/05-08/31/08

\$404,306

This award from the IMR_MIP program and the Office of Multidisciplinary Activity in to Florida State University supports a conceptual engineering design (CED) of a Free Electron Laser Light Source for High Magnetic Field Research. This project brings together the expertise of three world-leading US institutions; the National High Magnetic Field Laboratory, Tallahassee, home to the world's highest steady magnetic field, the Jefferson Laboratory, site of the most powerful free-electron laser, and the renowned University of California at Santa Barbara Center for Terahertz Science and Technology. In the first phase, experts from these laboratories will design a versatile and powerful free-electron laser facility plus the infrastructure to couple it to the Tallahassee high-field magnets. The free-electron laser system will provide unprecedented coverage of the electromagnetic spectrum in a single facility, producing radiation ranging from millimeter wavelengths to the near infrared. In spite of this great versatility, the new laser system will be based on tried and tested US technology, with reliability a key design factor. This high-magnetic-field plus free-electron-laser facility is being developed in response to emerging needs and desires of the scientific community, identified at a series of workshops and conferences in the past two years. It will be dedicated to new types of experiment in physics, chemistry and biophysics that utilize a magnetic field's ability to manipulate the electrons within matter, plus the free-electron laser's ability to probe the resulting changes as a function of time, laser power and wavelength. Such techniques promise to provide important information about materials ranging from semiconductors to DNA, and from superconductors to nanoparticles, and processes from quantum computation to photosynthesis. The provision of this unique facility will help to maintain the US's competitiveness in fundamental science and its spin-off emergent technologies. Students, and postdocs from a diverse demographic and institutional backgrounds will be participate in this CED project.

Mark Sherwin
DN Naval Research Laboratory, N00173-06-P-1198
Practical Terahertz Detectors
07/11/06-07/10/09
\$89,943

A practical THz detector for most earth-based applications would be one that is sufficiently sensitive to detect thermal THz emission with high signal to noise ratio in reasonable integration times, has modest cryogenic requirements, and is sufficiently fast for use as a heterodyne detector with wide intermediate frequency bandwidth, and for applications requiring high speed such as radar and communications. We propose to design, fabricate and test tunable antenna-coupled intersubband terahertz (TACIT) detectors and recently-conceived, closely-related plasmonic antenna-coupled Terahertz (PACT) detectors which operate at frequencies between 1 and 2 THz. These detectors are suitable for eventual incorporation into focal plane arrays.

Mark Sherwin
National Science Foundation, DMR-0703925
Terahertz Electro-Optics and Intersubband Micro-Plasmonics in Semiconductor Quantum Well Devices
07/01/07-06/30/10
\$390,000

This research program explores the response of semiconductor devices (designed and fabricated at UC Santa Barbara) in the "terahertz (THz) gap" of the electromagnetic spectrum between 0.1 and 10 THz. A frequency of 1 THz corresponds to 1 trillion (10¹²) cycles per second, 1000 times faster than the frequency at which cell phones broadcast, and 500 times lower than the frequency of green light. A new kind of detector for terahertz radiation will be explored, potentially useful for applications including security, medicine, and non-destructive materials testing. At the heart of this detector is a "gas" of electrons confined in a thin layer. The electrons will be forced perpendicular to the layer to search for the simultaneous existence of two stable operating states ("optical bistability," potentially useful as a terahertz-activated switch), spontaneous oscillation (a potential terahertz source) and a "chaotic" current induced by periodic driving (chaos is not normally observed in quantum mechanical systems). Strong terahertz radiation will also be used to enhance the functionalities of semiconductor optical devices, such as optical modulators used to transmit information over fiber-optic cables. Undergraduates, graduate students and post-doctoral researchers will receive broad experimental training. Along with the PI, they will bring novel outreach materials to local K-12 schools.

Mark Sherwin

S. James Allen

Elliott Brown

Song-I Han

Philip Lubin

Kevin Plaxco

Mark Rodwell

William M. Keck Foundation, SB080017

“Filming” Proteins in Action with UC Santa Barbara’s Free Electron Lasers

07/01/07-06/30/10

\$1,750,000

The movement and dynamics of proteins is of enormous importance in almost all of the biological processes and reactions that occur in living organisms. Unfortunately, however, our ability to characterize these motions is limited by the fact that proteins perform their biological roles in aqueous solution, a milieu that poses nearly intractable problems for established experimental methodologies to study molecular dynamics. Here we propose a research program dedicated to the hitherto difficult task of monitoring the collective, functional motions of proteins and other biomolecules in aqueous solution. The program will receive significant leveraging from UC Santa Barbara’s unique existing suite of high power terahertz free electron lasers. We will pioneer the development and application of two complementary techniques by which protein motions *in aqueous solution* can be “filmed:”

1. terahertz absorption spectroscopy of proteins and
2. terahertz pulsed electron paramagnetic resonance.

Taken together the two approaches will provide revolutionary insights into the dynamics of proteins as they function in their biologically relevant environments.

Mark Sherwin

National Science Foundation, DMR-0901970

Education and Outreach through Optical Terahertz Science and Technology

Workshop: Santa Barbara, California: March 2009

03/01/09-02/28/10

\$17,000

The recent development of terahertz (THz) technology based on optical light has resulted in rapid growth and real world applications. Prototype terahertz imaging systems have been installed in airports and post offices for security inspections. Industries from ship building to forestry are applying THz light for process monitoring. Biomolecular and biomedical research now experiment with terahertz technology. To ensure U.S. leadership in this rapidly moving field, it is essential that current science and engineering students become fluent in the technology. The Optical Terahertz Science and Technology

Workshop 2009 will achieve this through: a day of tutorials by specialists; three days of research presentations by world renowned investigators; and student poster presentations to be critiqued by leaders in the field. Undergraduate education will be impacted through a workshop on incorporating THz research into undergraduate teaching. The resulting modules will inspire undergraduates to participate in research that will give them the hands-on skills to pursue high tech careers and contribute to innovation in the U.S. economy. Three NSF divisions have contributed to supporting the attendance by graduate students and post docs at this workshop: the Division of Materials Research, the Division of Chemistry, and the Division of Electrical, Communications and Cyber Systems.

Mark Sherwin

Tanner Research Inc., UCSB FA9550-09-C-0161

A Room Temperature Tunable Antenna Coupled Intersubband Terahertz (TACIT) Detector for Man-Portable Spectroscopy

06/15/09-12/15/09

\$20,000

The Sherwin group at UC Santa Barbara will fabricate TACIT detectors and test their responsivity, noise and noise-equivalent power at temperatures between 4K and 300K. We will also perform a Phase I demonstration of the TACIT device, at an Air Force facility designated by the AFOSR POC (at an AFOSR customer site, for instance), whereby we will demonstrate the room temperature responsivity of the TACIT device to 1 THz radiation.

Dominik Stehr

Mark Sherwin

Pierre Petroff

DOE Los Alamos Area Office, RA2008A196

Time Resolved THz Spectroscopy in Semiconductor Quantum Posts

06/01/08-09/01/09

\$0

This project will investigate the electronic transitions in a new type of semiconductor nanostructure called quantum posts (QPs) which are closely related to quantum dots (QDs) but form a nanowire-like structure in the growth direction. Unlike in QDs, where the ground state transition in the semiconduction band is fixed around 50-60 meV, the transition energy related to the confinement in the z-direction is expected in the THz region in sufficiently “tall” QPs. Additionally, the transition energy is variable by changing the height of the QPs, allowing to address a large spectral range. This unique structure is currently successfully grown by MBE at UCSB and up to now, QPs with heights between 23 and 60 nm have been demonstrated with expected resonances between 16 meV (3.6 THz) and 2 meV (0.5 THz). In order to observe the THz resonances and part of their dynamics, we propose an all-optical

approach including an ultrafast interband excitation at the QP resonance followed by probing of the THz with single-cycle THz pulses with an adjustable delay. The approximately 15 nm broad interband resonance lies around 980 nm ((1.26 eV), requiring the use of a suitable ultrafast laser system at CINT.

Dominik Stehr Mark Sherwin

Pierre Petroff

DOE Los Alamos Area Office, C2008B072

Time Resolved THz Spectroscopy in Semiconductor Quantum Posts

06/01/08-09/01/09

\$0

This project will investigate the electronic transitions in a new type of semiconductor nanostructure called quantum posts (QPs) which are closely related to quantum dots (QDs) but form a nanowire-like structure in the growth direction. Unlike in QDs, where the ground state transition in the semiconduction band is fixed around 50-60 meV, the transition energy related to the confinement in the z-direction is expected in the THz region in sufficiently “tall” QPs. Additionally, the transition energy is variable by changing the height of the QPs, allowing to address a large spectral range. This unique structure is currently successfully grown by MBE at UCSB and up to now, QPs with heights between 23 and 60 nm have been demonstrated with expected resonances between 16 meV (3.6 THz) and 2 meV (0.5 THz). In order to observe the THz resonances and part of their dynamics, we propose an all-optical approach including an ultrafast interband excitation at the QP resonance followed by probing of the THz with single-cycle THz pulses with an adjustable delay. The approximately 15 nm broad interband resonance lies around 980 nm ((1.26 eV), requiring the use of a suitable ultrafast laser system at CINT.

Galen Stucky

Environmental Protection Agency, SB060043

US EPA Fellowship

08/03/05-08/02/08

\$49,351

The objective of this proposal is the understanding and development of inorganic materials with compositions and nanostructures optimized for the coupling of energy from sunlight to oxidation/reduction chemistry for the photoelectrochemical degradation of environmental pollutants.

Contracts/Grants Awarded 2008-2009

Air Force

Michael Bowers
FA9550-06-1-0069 01/01/06-11/30/09 \$ 189,000
POSS and Metal Clusters: Structures and Energetics

Department of Energy

Los Alamos Area Office

Dominik Stehr, Mark Sherwin, Pierre Petroff
RA2008A196 06/01/08-09/01/09 \$ 0
Time Resolved THz Spectroscopy in Semiconductor Quantum Posts

Dominik Stehr, Mark Sherwin, Pierre Petroff
C2008B072 02/01/09-02/01/10 \$ 0
Time Resolved THz Spectroscopy in Semiconductor Quantum Posts

Miscellaneous Offices and Programs

Steven Buratto, Michael Bowers
DE-FG02-06ER15835 09/01/07-08/31/10 \$ 168,736
Chemical Imaging with 100nm Spatial Resolution

Department of Energy Subtotal \$ 168,736

Jet Propulsion Laboratory

Philip Lubin
1367008 02/10/09-09/30/13 \$ 10,000
Planck Educational and Public Outreach Effort at UCSB

Philip Lubin
1367008 02/10/09-09/30/13 \$ 10,000
Planck Educational and Public Outreach Effort at UCSB

Philip Lubin
1372889 04/06/09-05/30/09 \$ 12,000
W-Band Amplifier Assemblies

Jet Propulsion Laboratory Subtotal \$ 32,000

National Aeronautics & Space Administration

David Cannell
NNX08AE53G 03/01/08-02/28/2010 \$ 60,000
Gradient Driven Fluctuations

National Science Foundation

Guenter Ahlers

DMR-0702111 05/01/07-04/30/10 \$ 155,000

Turbulent Convection in a Fluid Heater from Below

Steven Buratto, Michael Bowers, Horia Metiu

CHE-00749489 04/01/08-03/31/10 \$ 167,000

Model Nanocluster Catalysts: The Role of Size, Shape and Composition on the Catalytic Activity on Monometallic, Bimetallic and Metal Oxide Clusters on Oxide Surfaces

Deborah Fygenson, Dirk Bouwmeester

CCF-062257 09/01/06-08/31/09 \$ 100,000

DNA Patterned Pairs of Colloidal Quantum Dots: A Scalable Approach to Computing Without Wires

Songi Han, Frederick Dahlquist, Mark Sherwin

CHE-0821589 08/01/08-07/31/11 \$1,254,623

Bruce Lipshutz

CHE-0550232 02/01/06-01/31/10 \$ 148,000

Asymmetric Catalysis with Ligated Copper Hydride

Mark Sherwin

DMR-0703925 07/01/07-06/30/10 \$ 130,000

Terahertz Electro-Optics and Intersubband Micro-Plasmonics in Semiconductor Quantum Well Devices

Mark Sherwin

DMR-0901970 03/01/09-02/28/10 \$ 17,000

Education and Outreach through Optical Terahertz Science and Technology

National Science Foundation Subtotal \$1,971,623

National Institutes for Health

National Institute of General Medical Sciences

Frederick Dahlquist

R56 GM059544 08/01/08-07/31/09 \$ 290,250

New Reactions for Direct, Native Peptide Ligations

UC Los Angeles

Michael Bowers

SB070075 09/01/06-07/31/09 \$ 255,168

Pathogenic Protein Folding and Human Disease

Research Support Summary (2008-2009)

% Total

Federal			
Air Force	189,000	7%	6.37%
Department of Energy	168,736	6%	5.69%
Jet Propulsion Laboratory	32,000	1%	1.08%
National Aeronautics and Space Administration	60,000	2%	2.02%
National Science Foundation	1,971,623	73%	66.46%
National Institutes for Health	290,250	11%	9.78%
Federal Totals	\$2,711,609	100%	91.40%
State			
UC Discovery Grant	0	0%	0.00%
University of California, Los Angeles	255,168	100%	8.60%
State Totals	\$255,168	100%	8.60%
TOTALS	\$2,966,777		100.00%

Charts and Graphs

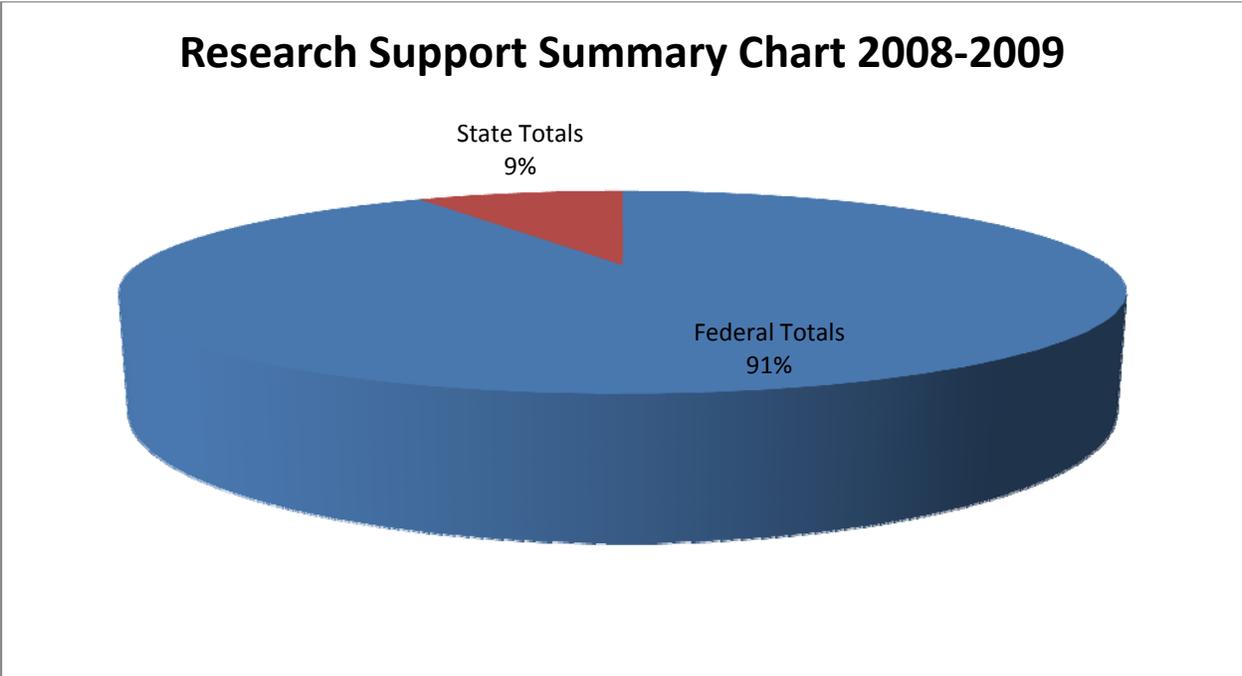


Chart 1: Research Support Summary Chart 2008-2009

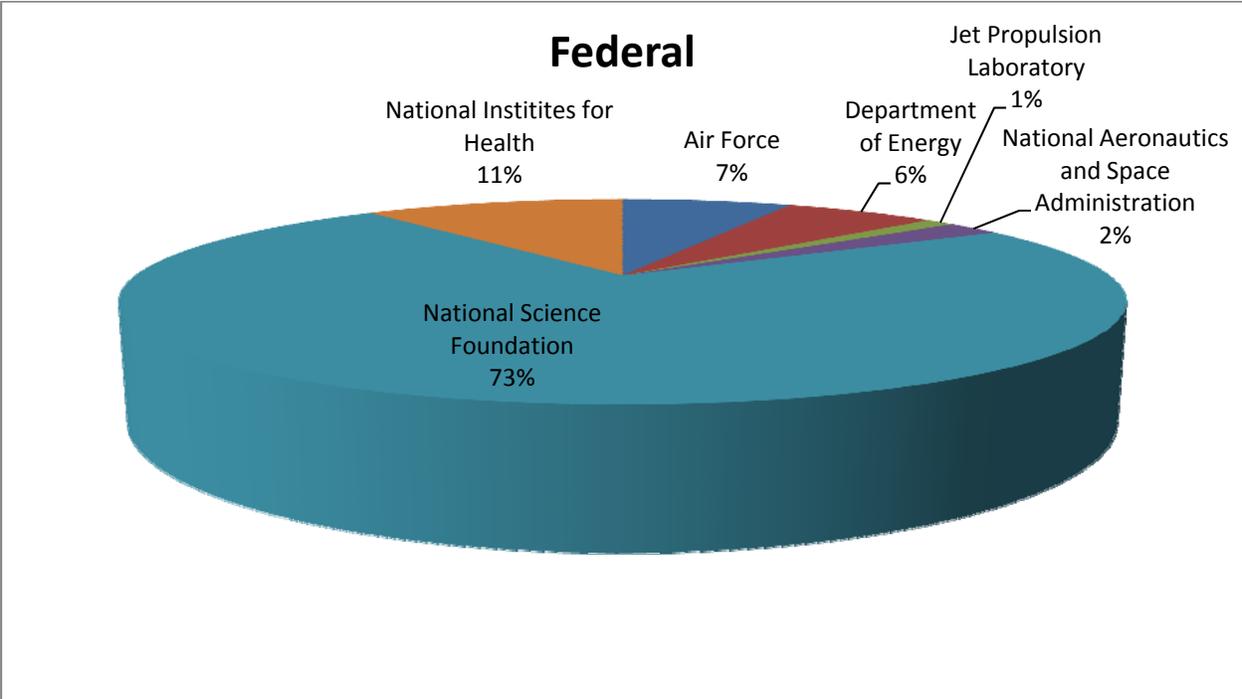


Chart 2: Federal Research Support Summary Chart

State

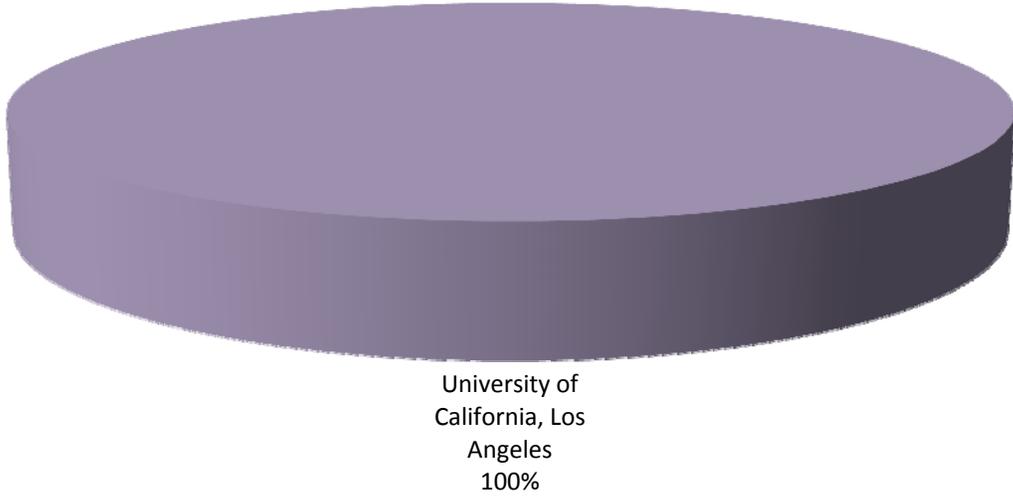


Chart 3: State Research Support Summary Chart

Base Budget and Overhead Generated (thousands of dollars)

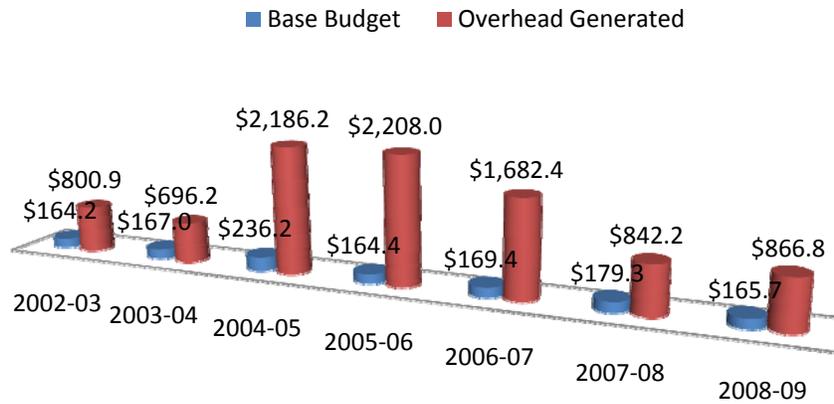


Chart 4: Base Budget and Overhead Generated

Number of Proposals Submitted and Funded

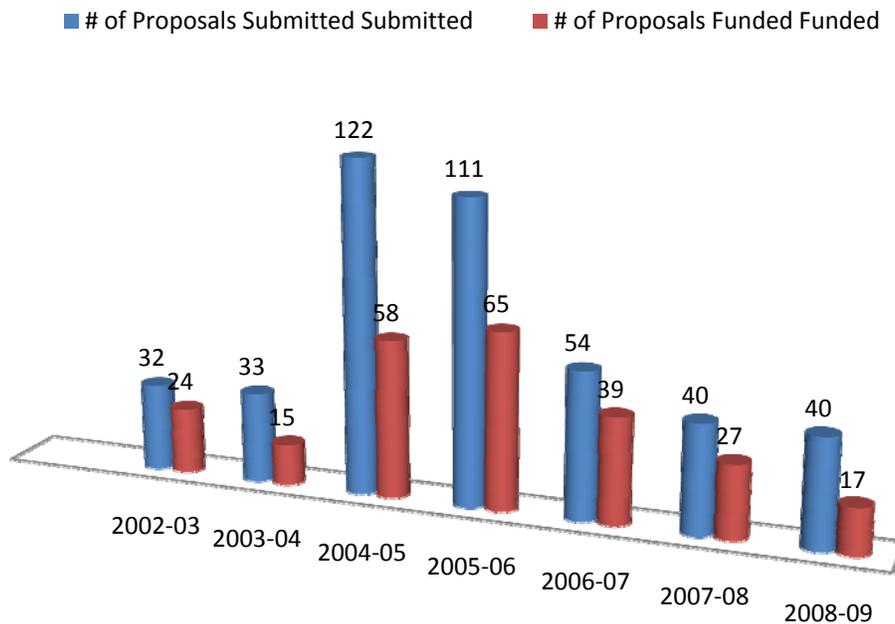


Chart 5: Number of Proposals Submitted and Funded

Value of Proposals Submitted and Funded (millions of dollars)

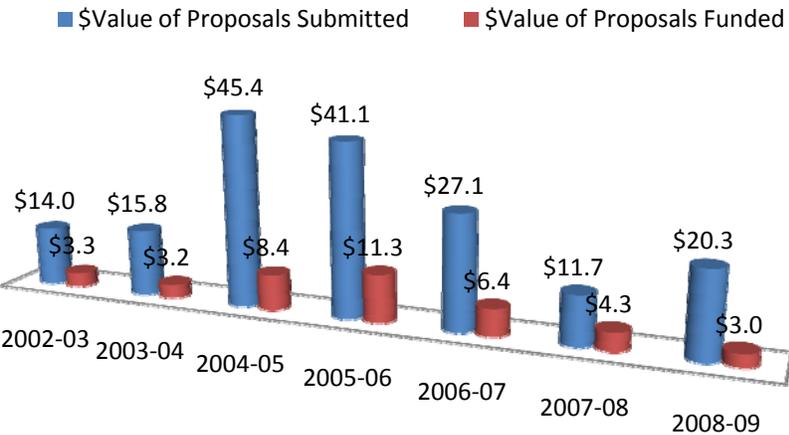


Chart 6: Value of Proposals Submitted and Funded

Number of Awards Administered

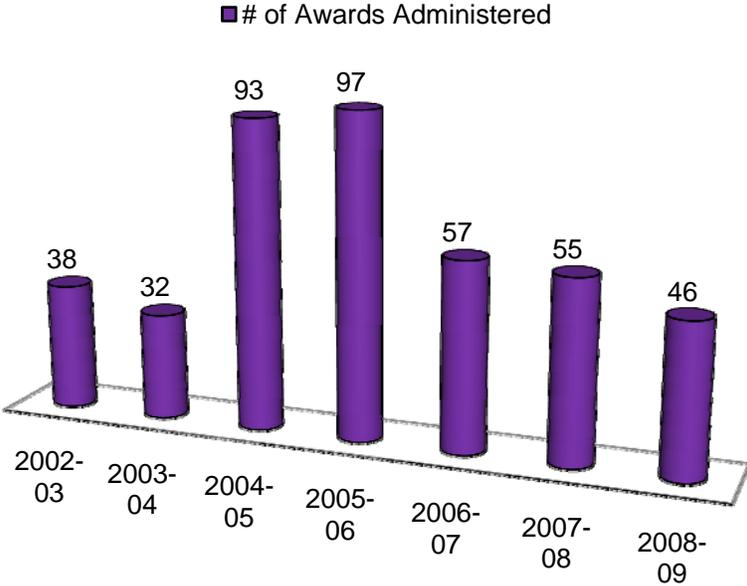


Chart 7: Number of Awards Administered

**Value of Contracts and Grants Administered
(millions of dollars)**

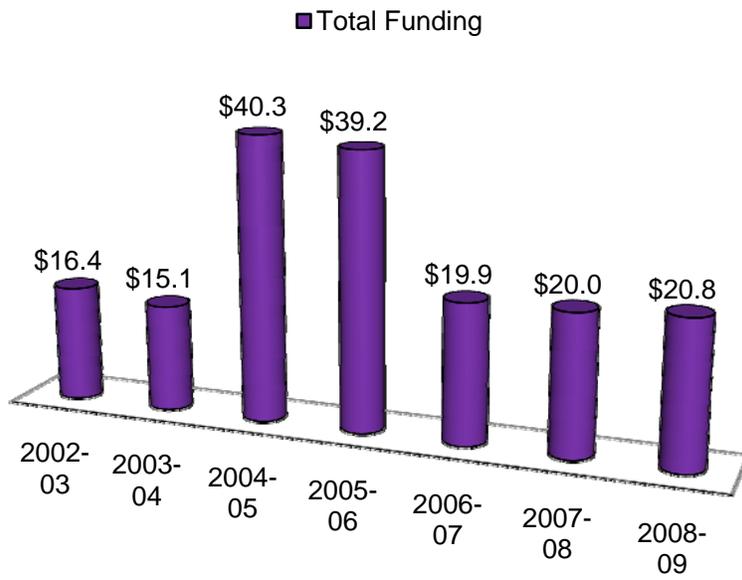


Chart 8: Value of Contracts and Grants Administered

Statistical Summary for ITST

2008-2009

1. Academic personnel engaged in research:	
a. Faculty	25
b. Professional Researchers (including Visiting)	5
c. Project Scientists	7
d. Specialists	6
e. Postdoctoral Scholars	14
f. Postgraduate Researchers	0
TOTAL	57
2. Graduate Students:	
a. Employed on contracts and grants	37
b. Employed on other sources of funds	0
c. Participating through assistantships	0
d. Participating through traineeships	0
e. Other (specify)	0
TOTAL	37
3. Undergraduate Students:	
a. Employed on contracts and grants	9
b. Employed on other funds	1
c. Number of volunteers, & unpaid interns	11
TOTAL	21
4. Participation from outside UCSB: <u>(optional)</u>	
a. Academics (without Salary Academic Visitors)	1
b. Other (2 high school students + 1 chief scientist, industry)	3
5. Staff (Univ. & Non-Univ. Funds):	
a. Technical	9
b. Administrative/Clerical	4
6. Seminars, symposia, workshops sponsored	23
7. Proposals submitted	40
8. Number of different awarding agencies dealt with*	31
9. Number of extramural awards administered	46
10. Dollar value of extramural awards administered during year**	\$20,469,299
11. Number of Principal Investigators***	30
12. Dollar value of other project awards ****	\$643,960
13. Number of other projects administered	10
14. Total base budget for the year (as of June 30, 2009)	\$165,727
15. Dollar value of intramural support	\$835,233
16. Total assigned square footage in ORU	10,582
17. Dollar value of awards for year (08 Total)	\$2,966,777

* Count 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	Professor	Physics
S. James Allen	Professor	Physics
Bjorn Birnir	Professor	Mathematics
Jeffrey Bode	Assistant Professor	Chemistry and Biochemistry
Dirk Bouwmeester	Professor	Physics
Michael Bowers	Professor	Chemistry and Biochemistry
Elliot Brown	Professor	Electrical and Computer Engineering
Steven Buratto	Professor	Chemistry and Biochemistry
David Cannell	Professor	Physics
Nancy Carrillo	Graduate Student	Chemistry and Biochemistry
Bradley Chmelka	Professor	Chemical Engineering
Andrew Cleland	Professor	Physics
Lawrence Coldren	Professor	Electrical and Computer Engineering
Frederick Dahlquist	Professor	Chemistry and Biochemistry
Deborah Fyngenson	Associate Professor	Physics
Song-I Han	Assistant Professor	Chemistry and Biochemistry
Robert Jacobs	Professor	Pharmacology, Ecology, Evolution & Marine Biology
Lipshutz	Professor	Chemistry and Biochemistry
Dan Little	Professor	Chemistry and Biochemistry
Philip Lubin	Professor	Physics
Horia Metiu	Professor	Chemistry and Biochemistry
Pierre Petroff	Professor	Materials
Kevin Plaxco	Professor	Chemistry and Biochemistry
Craig Pryor	Chief Scientist	Terahertz Device Corporation
Mark Rodwell	Professor	Electrical and Computer Engineering
Douglas Scalapino	Research Professor	Chemistry and Biochemistry
Mark Sherwin	Professor	Physics
Dominik Stehr	Postdoctoral Scholar	Physics
Galen Stucky	Professor	Chemistry and Biochemistry
Jelena Vuckovic	Assistant Professor	Stanford University

Map

Take a left at the elevator then down the hall to room 3410

Our offices are located on the 3rd floor of Broida Hall

