2013-2014

INSTITUTE FOR TERAHERTZ
SCIENCE AND TECHNOLOGY

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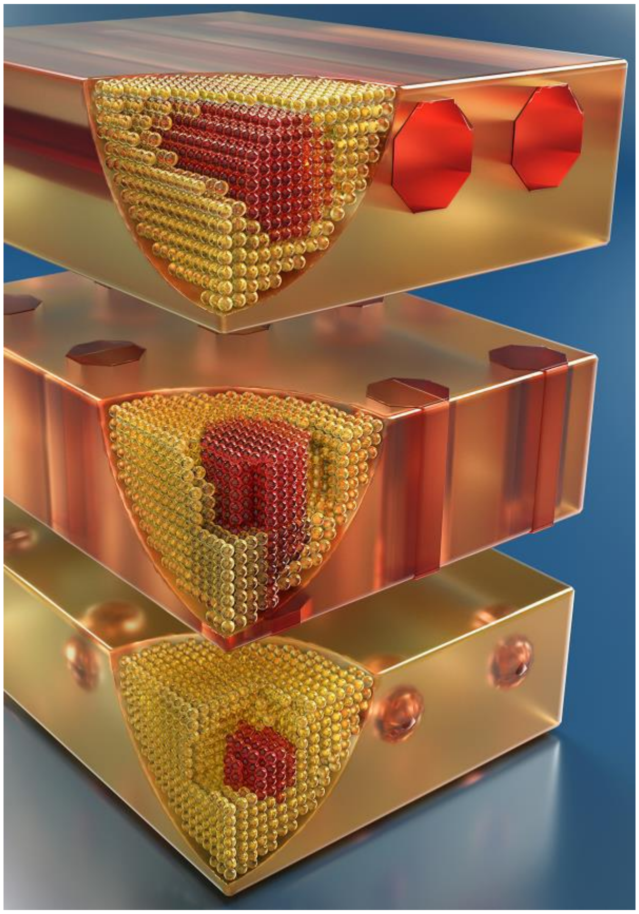
ANNUAL REPORT



Dr. Mark Sherwin, Director | Rita Makogon, Manager
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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.

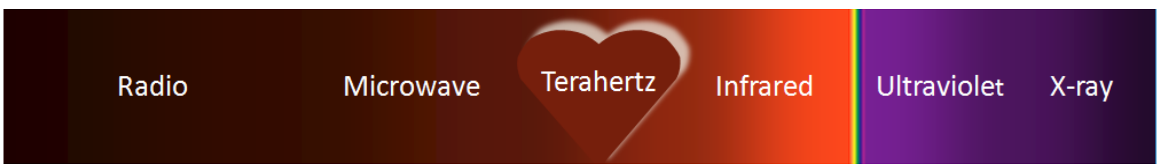


Figure 1: Chart showing ITST's research emphasis at the heart of the electromagnetic spectrum.

*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.

Director's Statement

The over-arching goal of the strategic plan of Institute for Terahertz Science and Technology (ITST) is to maximize the impact of its unique facilities and personnel on the campus, national and international stages. We have made significant progress towards this goal over the last year. Highlights include

- Dr. Nick Agladze joined ITST as its "Principal Experimentalist." He began in August 2013, coming from Cornell University where he distinguished himself with over 20 years of developing custom instrumentation for infrared and terahertz spectroscopy, including unique new spectrometers. He has had a strong and immediate impact on ITST, jumping in to our challenging FEL development effort, designing and setting up experiments for outside users, and troubleshooting/solving many instrumentation problems for ITST-affiliated research groups.
- A SEED grant from the UCSB Materials Research Science and Engineering Center (MRSEC) was awarded to the director, with the goal of bringing the unique tools of ITST to bear on important problems in materials research. In particular, the SEED grant is supporting the development of methods to rapidly measure the electrical conductivity of a wide variety of materials without the need for making electrical contacts to them.
- Supported by a grant from the NSF, the 30-year old accelerator that drives the UCSB Free-Electron Lasers (FELs) has been torn apart and rebuilt, mostly by Mr. David Enyeart, ITST's remarkably talented Senior Development Engineer. This was a necessary and large endeavor that was not guaranteed to succeed. The upgrade lasted 9 months, ending in September 2014. I am delighted to report that the accelerator is working better than it ever has, and the UCSB FELs are producing science once again.

ITST has also seen the addition of several new users, both internal and external to UCSB. Since the FEL has been down for the accelerator upgrades, these users have been doing experiments with ITST's other unique instruments. The following new projects have begun using the ITST's home-built electron paramagnetic resonance (EPR) spectrometer, which operates at 240 GHz (0.24 THz) as opposed to the usual 10 GHz:

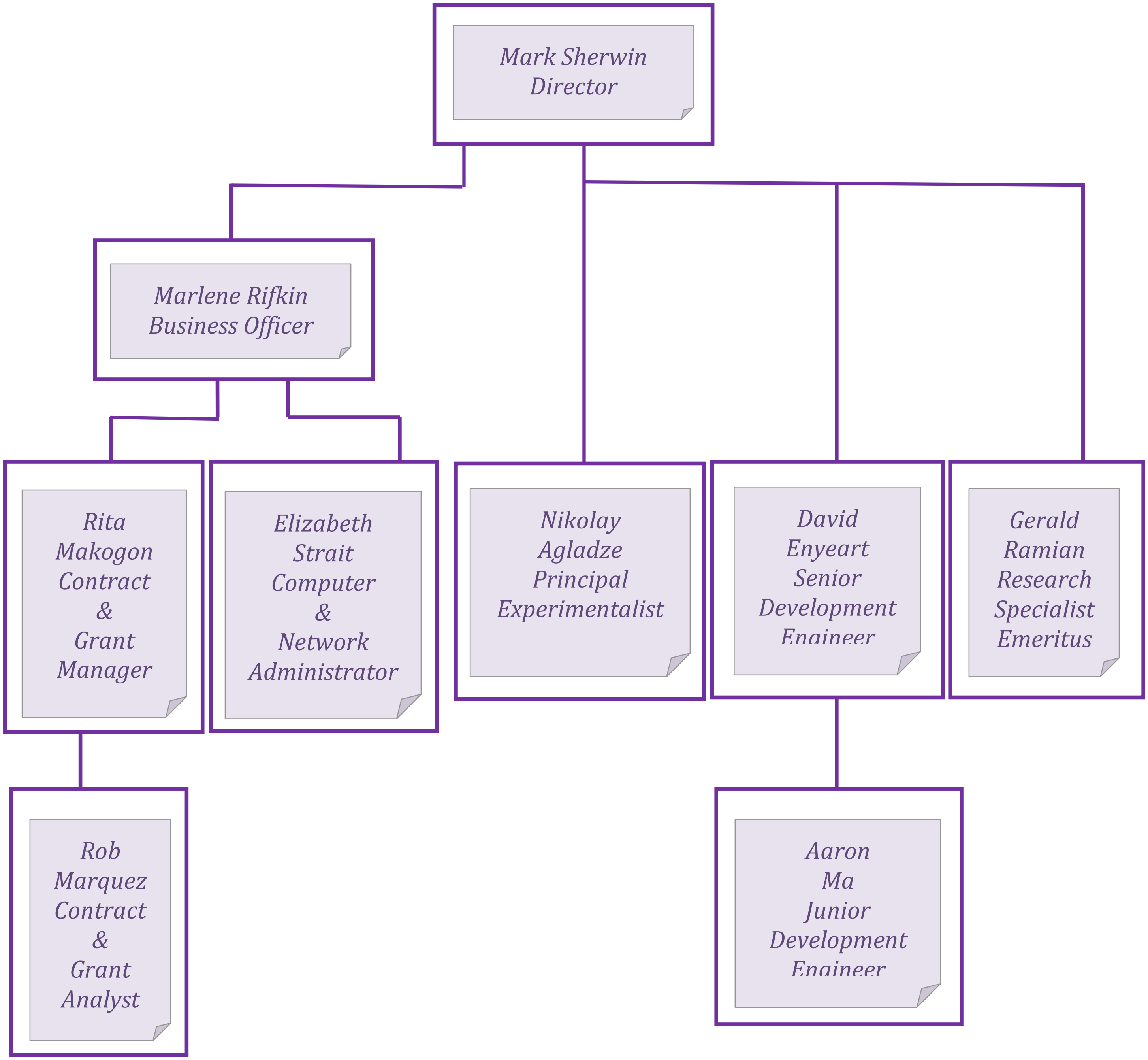
- Prof. Sophia Hayes from Washington University in St. Louis, studying 240 GHz EPR on impurities in GaAs.
- Ms. Melanie Drake, Ph. D. student in Chemical Engineering from the group of Prof. Jeff Reimer at UC Berkeley, has studied the properties of impurities in diamond. Profs. Hayes and Reimer are both NMR spectroscopists and professional colleagues of ITST Advisory Committee Chair Prof. Song-I Han, who piqued their interest sufficiently to bring them to UCSB.
- Mr. Yonghau (Steven) Zheng, a Ph. D. student of Prof. Fred Wudl, has measured the EPR spectrum of a surprising new radical he has synthesized.

We look forward to increasing numbers of new users now that the FELs are back in operation, including upcoming visits from researchers from Harvard University.

On the administrative side, there have also been large changes in ITST. In particular, Ms. Marlene Rifkin, the business officer of this ORU since 2000, retired at the end of June 2014. It is no exaggeration to state that ITST would not be here today were it not for Marlene's tremendous energy, organizational genius and financial acumen. She has left ITST in tremendous shape, with an extremely well-trained and talented staff. Ms. Rita Makogon has taken over the administrative leadership of ITST. It is a great testament to Marlene and all of the ITST staff—Rita, Mr. Rob Marquez, and Ms. Elizabeth Strait,—that the transition has been virtually seamless. We all miss Marlene, but the ITST contracts and grants management operation has continued to provide its usual level of outstanding customer service.

We are all looking forward to the challenges ahead.

Organizational Chart



Advisory Committee

Song-I Han	**Chemistry and Biochemistry, Committee Chair**
S. James Allen	Former iQuest Director, Physics
Andrew Cleland	Physics
Ania Jayich	Physics
Ben Mazin	Physics
Christopher Palmstrom	Materials &Electrical and Computer Engineering
Kevin Plaxco	Chemistry and Biochemistry
Jon Schuler	Electrical and Computer Engineering
Wim Van Dam	Computer Science

Ex Officio Members

Rick Dahlquist	Chair, Chemistry and Biochemistry
Fyl Pincus	Chair, Physics
Marlene Rifkin	Business Officer, ITST
Mark Sherwin	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

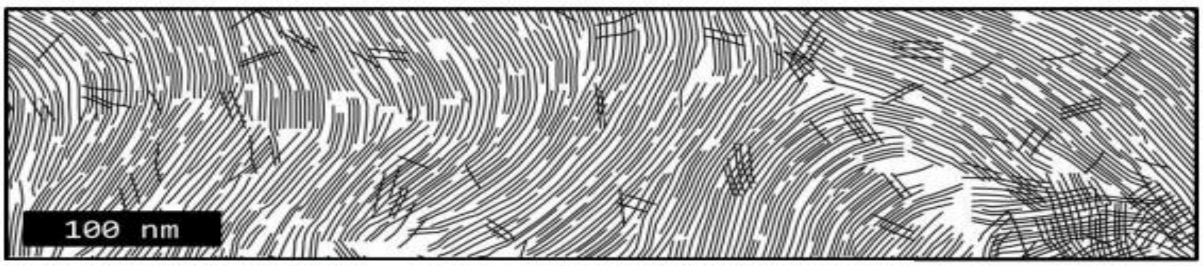
Technical Staff-ITST

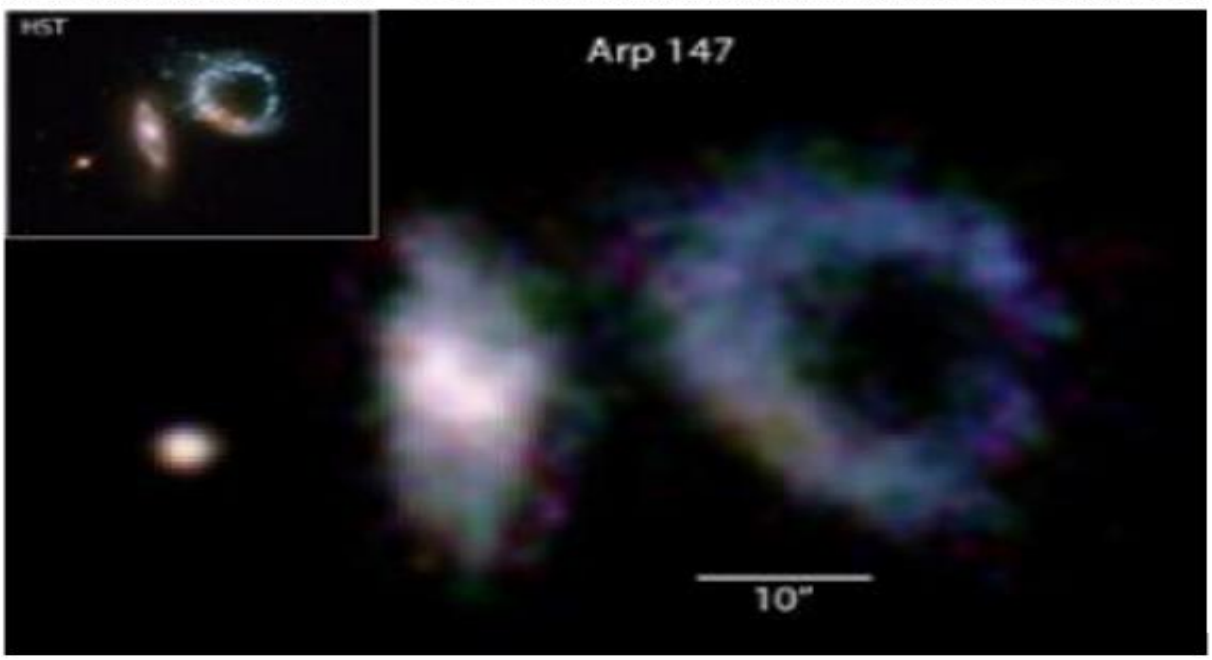
Nick Agladze, Principal Experimentalist
David Enyeart, Senior Development Engineer
Aaron Ma, Junior Development Engineer
Gerald Ramian, Research Specialist Emeritus

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:





12/05/13:
Distance measurements in biomolecules using Gd3+ spin labels - pros and cons: Daniella Goldfarb, The Erich Klieger Professorial Chair in Chemical Physics, Weizmann Institute of Science

01/09/14
Long-range order and unusual packing motifs in high-performance organic semiconductors: Christopher J. Takacs, Materials Department, University of California Santa Barbara

01/16/14:
Astronomy by way of Condensed Matter Physics: Ben Mazin, Physics Department, University of California, Santa Barbara

01/23/14:
Sub-mm-Wave Technologies: Systems,ICs, THz transistors: Mark Rodwell, ECE Department, University of California Santa Barbara

01/31/14:
The Enzymatic Mechanism of Oxalate Decarboxylase Investigated by EPR: Alexander Angerhofer, Department of Chemistry, University of Florida

02/06/14:
Electric Field Screening of Carbon Fiber Cathodes: Don Shiffler, Air Force Research Laboratory, Directed Energy Directorate, Albuquerque, New Mexico

02/13/14:
Induced magnetism and control of quantum critical behavior in perovskite quantum wells: Clayton Jackson, Materials Department, UCSB

02/20/14:
Nuclear polarization from nitrogen vacancy ensembles in diamond: Melanie Drake, Department of Chemical and Biomolecular Engineering, UC Berkeley

03/06/14:
THz metamaterial waveguides and lasers: Benjamin Williams, Department of Electrical Engineering, UCLA

04/03/14:
A Hubbard view for correlated hydrogen bonds: Fyl Pincus, Physics Department, UCSB

04/10/14:
Nanoscale magnetic imaging with a single spin in diamond: Bryan Myers, Jayich Group, Physics Department, UCSB

04/17/14:

Fabrication and characterization of gate-defined structures in epitaxially grown InAs heterostructures: Javad Shabani, Electrical and Computer Engineering, UCSB, Palmstrøm group

04/24/14:

Nano- and opto-mechanics of fully self-assembled nanowires: Martino Poggio, Physics Department, University of Basel

05/08/14:

Nuclear hyperpolarization: The Quest for Ultra-High Sensitivity NMR, Quantum Computing, and Nuclear Spintronics: Jeff Reimer, UC Berkeley

05/15/14:

Development of high-frequency EPR spectrometer and investigation of impurities in nanodiamonds: Cho Franklin, USC, Takahashi group

05/22/14:

Using dynamic nuclear polarization enhanced NMR techniques to understand heterogeneous solid materials: Rahul Sangodkar, Chemical Engineering UCSB, Chmelka & Doherty Research Groups

06/05/14:

Room-temperature operating semiconductor-based THz sources and detectors: Sascha Preu, Technical University Darmstadt, Germany

06/19/14:

Assignment of quantum well electronic states of 69Ga OPNMR of GaAs/AlGaAs: Prof. Sophia Hayes, Washington University, Department of Chemistry

Awards Administered

(July 2013 – June 2014)

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-1158514
Turbulent Convection in a Fluid Heated from Below
06/01/12-05/31/16
$480,000 (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 heat-transport devices in computer applications to the giant cooling systems of power plants. And yet much 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
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
$370,000 ($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.

Dirk Bouwmeester
National Science Foundation, PHY-1314982
Implementing a Quantum CNOT Gate Using Solid State Cavity QED
09/01/13-08/31/16
$90,000 ($270,000)

By combining single-photon technology with semiconductor electro-optical devices we investigate a scheme for a quantum CNOT gate. Such a gate is a fundamental building block of quantum computers and quantum communication systems. Nanofabrication and material-growth concepts will be implemented to create optical micro cavity structures with embedded artificial atoms in the form of a nanoscale semiconductor structure, called a quantum dots. A quantum dot, if positioned at the center of the cavity and at the cavity resonant frequency, will interact with an incoming photon in such a way that the photon polarization will become entangled with the electronic state of the quantum dot. This interaction establishes the quantum CNOT gate; the quantum state of the photon is changed depending on the quantum state of the electron.

The research topic directly relates to the micro optoelectronics industry as well as to fundamental studies of confined electron properties in semiconductors. Potential applications in classical and quantum information storage and processing are expected to follow from this project. Since the interactions are at the single photon level, the devices will in principle be very energy efficient. It should however be mentioned that this study does require low-temperature operation conditions. Alternative implementations based on different cavity designs and different optical emitters that remain active a room temperature will also be considered.

Michael Bowers
National Science Foundation, CHE-0909743
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
$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
7/1/12-01/11/15
$269,309

A request is made is transform a currently existing instrument onto one capable of studying mass-selected 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.

Michael Bowers
National Institute of Health 1 R01 AG047116-01
Amyloid β-Protein: Wild Type and Familial Mutant Assembly and Inhibition
09/01/13-06/30/17
$441,176 ($1,768,028)

The overarching goal of our research is to determine the molecular basis for amyloid β-protein's contribution to Alzheimer's disease. Specifically we intend to measure early oligomer-size distributions of a series of natural and intentionally mutated Aβ40, Aβ42 and tau fragment peptides, determine their structures and use this information to establish the aggregation mechanism. In parallel, we will investigate the effect of a series of aggregation inhibitors on this process to obtain their inhibition mechanism and evaluate their suitability as potential therapeutic agents. Finally, we will investigate the general mechanism of peptide aggregation using a series of model peptides. We will use ion-mobility-based mass spectrometry (IMS-MS) experimental methods coupled to high-level molecular dynamics simulations in pursuing these goals. My group has pioneered the modern development of IMS-MS and its application to complex macromolecular systems. We first used it to unravel the size-specific structural evolution of carbon cluster growth in arcs, leading to the characterization of the mechanism for fullerene formation. More recently we have focused on aggregating biological systems including prions (mad cow and other TSE diseases), α-synuclein (Parkinson's disease), hIAPP (type 2 diabetes) and amyloid β-protein. This work has depended on complementary high-level simulations which will continue. We feel the excellent progress made to date on Aβ peptides and on other amyloid systems strongly indicates our ability to successfully achieve the goals set out in The Specific Aims of this proposal.

Michael Bowers
National Science Foundation NSF CHE-1301032
Peptide Assembly: Mechanism and Inhibition
09/01/13-08/31/16
$495,000

The award CHE-1301032 provided by the Chemical Structure, Dynamics and Mechanism-B Program (CSDM-B) and the Chemistry of Life Processes of the National Science Foundation to Professor Michael T. Bowers at the University of California at Santa Barbara will be used to investigate the mechanism of peptide assembly. This is currently a very active area of research both for its fundamental importance and because of possible therapeutic applications in neurological diseases. These studies will include the determination of oligomer distributions, the structures of sized selected oligomers and the effect of select inhibitors on this process. Peptides will be selected to test existing models for beta sheet formation and eventual fibrilization and for their possible implications in amyloid based diseases. Experimental methods will include ion mobility spectrometry coupled with mass spectrometry, atomic force microscopy and transmission electron spectroscopy and a newly developed oligomer size selected infrared spectroscopy experiment constructed at the Fritz Haber Institute in Berlin, Germany. The experiments will be complimented by high level theoretical calculations including both DFT and replica exchange molecular dynamics. Inhibitors will include both naturally occurring substances like polyphenols and specially synthesized molecules designed for select peptide attachment.

The two fastest growing major diseases in the US today are Alzheimer's disease and Type 2 Diabetes. These seemingly dissimilar diseases share the common trait of having toxic agents that come from the assembly of ordinarily innocuous agents (peptides) in the body: one process occurring in the brain causing Alzheimer's disease and the other in the pancreas causing Type 2 Diabetes. It isn't clear how these normally safe species assemble into deadly ones nor is it clear how they kill cells once they do assemble. This is a difficult problem to study with the normal tools of biochemistry that can't select specific assembled peptides and hence can't tell their structure or how toxic they are. The thrust of this proposal is to provide a new set of methods that can do this selecting and to apply these methods to model peptide systems to learn the factors that control peptide assembly in general and then test simple molecules that can stop this assembly in its tracks. Finally the results are translated into presentations that can be given to local high schools and each Bowers group member visits several such schools each year to make these presentations.

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 (SO_3H) 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.

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
09/01/11-05/31/14 (05/31/15)
$849,157 (1,101,093)

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.

Bruce Lipshutz
NOVARTIS Pharmaceutical SB140127
New Methodologies in Synthesis Using Micellar Catalysis
06/15/14-06/15/15
$182,000

The goal is to develop environmentally benign methods that avoid use of organic solvents as the traditional reaction medium. A postdoctoral student will be hired to develop a variety of new methodologies that rely on nanoreactors formed in water using surfactant technology developed in the group. New Synthetic methodologies in the following fields could be investigated:

Iron-mediated chemistry
Ullman-type chemistry
Oxidation methodologies
Reduction methodologies
Organometallic chemistry (organozincates, others)
Amide bond formation – extension of scope where potential epimerization, catalytic methods
Selective carboxyl reduction methods
C-N bond-formation transformations
Chemistry of highly energetic compounds (nitroalkanes, azides, nitration…)
Gas-mediated transformations (hydrogenations, hydroformylation, hydrocarbonylation…)

.

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.

Philip Lubin
Freedom Photonics LLC SB140070
Freedom Photonics Atmospheric Modeling
12/01/13-09/30/14
$18,388

UCSB will support aid in the development of atmospheric modeling in the infrared to explore the issues of transmission of IR wavelengths through varying atmospheric conditions such as fog, rain etc. In particular we will explore the ability to transmit information in the 1550 nm range. Primary emphasis will be placed on horizontal paths from 0.1 to 10 Km. Typically we will compute to level of down to 10^{-4} in transmission.

1) Study of atmospheric transmission from 0.3 to 15 microns with varying amounts of fog.
2) Study the sensitivity of transmission to varying rates of rain and raindrop sizes.
3) Study the sensitivity the sensitivity of transmission to varying conditions of dust.
4) Study atmospheric radiance for the above.
5) Study optimal IR atmospheric windows.
6) Plots and summaries will be prepared for all of the above.
7) Study atmospheric scintillation (seeing) effects to determine relevancy.

Philip Lubin
Raytheon Company SB140137-0001
Task 1: Advanced Camera Development
04/01/14-12/31/14
$67,000

Software development on Xilinx Zynq based FPGA/ ARM core

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.

Douglas Scalapino
Oak Ridge National Laboratory, 4000129396
Studies of the Properties of Strongly Correlated Materials
04/14/14-03/31/15 (03/31/16)
$127,758 ($253,802)

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
Song-I Han
U.S.-Israel Binational Science Foundation 2010130
Development of Gd^{3+}-Based Spin Labels for Probing Structure, Dynamics and Interfaces by Electron Paramagnetic Resonance Techniques
10/01/11-09/30/14 (09/30/15)
$69,395 (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 for EPR and DNP. Using a variety of mono- and bis-Gd^{3+} 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 Gd^{3+} concentration. Having established a good understanding of the spin dynamics that is needed for the optimum measurements conditions and the design of appropriate Gd^{3+} chelators we will explore Gd^{3+} spin labels for structure determination through Gd^{3+}-Gd^{3+} distance measurements and their potential to probe protein dynamics and light triggered conformational changes. Finally, we propose to develop a Gd^{3+} spin label based methodology to study polymer interfaces in systems with nanometer scale heterogeneities and phase boundaries using solid state DNP of ^{1}H and natural abundance ^{13}C 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
10/01/11-09/30/15
$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 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 GD^{3+} -Based Spin Labels for Structural Studies of Membrane Proteins
01/01/13-12/31/15
$600,720 ($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 ½ 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 7/2 Gd^{3+} ion. The attributes of nitroxide and Gd^{3+} -based spin labels are very different and make them optimal for environments that are largely complementary. In particular, the Gd^{3+} 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 Gd^{3+} 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 Gd^{3+} ion are particularly favorable at high magnetic fields and frequencies, one of the frontiers of EPR. The development of Gd^{3+} 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.

Mark Sherwin
University of Pittsburgh 2013PR0455
07/31/13-07/30/16
$346,875

Sherwin/UC Santa Barbara will hire 1 graduate student researcher for the duration of this proposal. They will perform the following tasks:

1) *Measure x3 and x5 frequency multiplication from CVD graphene:* Illuminate CVD graphene sample with ~1 kW pulses from the UCSB free-electron lasers tuned to a frequencies near (a) 0.6 THz and (b) 3 THz. For case (a), measure output at 1.8 and 3 THz. For case (b) measure output at 9 and 15 THz.
2) *Construct a spectrometer to measure high-order frequency multiplication:* We will construct a spectrometer which is capable of measuring frequency multiplication of 0.6 THz by more than a factor of 10.
3) *Design and fabricate slot antennas to enable high-order harmonic generation from subwavelength size (~10 µm) samples.* Exfoliated graphene samples and patterned GCO structures are considerably smaller than the wavelength of terahertz radiation. A simple slot antenna will enable effective coupling to study harmonic generation from samples with ~10 µm dimensions.
4) *Measure Terahertz harmonic generation from mechanically-exfoliated graphene flakes*. Flakes will be placed in slot antennas, then terahertz harmonic generation experiments will be performed.

Measure plasmon-enhanced harmonic generation from GCO nanostructures. GCO nanostructures will be patterned by Levy group and inserted into slot antennas. These structures will be sent to UCSB for measurements of frequency multiplication.

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
$407,415 ($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.

Jatila van der Veen
PARAGON TEC
NASA Summer of Innovation: Planck Mission Education and Outreach
07/01/13-08/15/13
$2,500

The NASA Summer of Innovation (SoI) program was started by the Obama Administration in 2010 to provide seed money for improving science education, aimed specifically at the middle school level, through existing summer and/or afterschool programs. In June, 2013 Dr. Jatila van der Veen received a small ($2500) NASA SoI award as a supplement to her existing NASA Planck Mission Education and Public Outreach program. The purpose of the award was to provide professional development for two local middle school science teachers by funding them to work in the Experimental Cosmology Lab during July and August, 2013, and then help them develop appropriate science curricula based on their summer research experiences. Thus it falls under the categories of public service and supplemental funding to an existing program, as described in the statement of Campus Vital Interest. Overhead is already being drawn from Dr. van der Veen's NASA/Planck Mission award.

Contracts/Grants Awarded 2013-2014

DAF Office of Scientific Research

Michael Bowers
FA2386-12-1-3011 06/15/11-06/14/15 $ 240,000
Litigated Metal Clusters: Structures, Energetics and Reactivity

DAF Office of Scientific Research Subtotal $ 240,000

Freedom Photonics LLC

Philip Lubin
SB140070 12/01/13-09/30/14 $ 18,388
Freedom Photonics Atmospheric Modeling

Freedom Photonics Subtotal $ 18,388

Jet Propulsion Laboratory

Jatila van der Veen
1388406 10/01/09-03/11/2015 $ 92,700
The Planck Visualization Project: Education and Public Outreach Effort of the U.S. Plank Mission

Jet Propulsion Laboratory Subtotal $ 92,700

NIH National Institute on Aging

Michael Bowers
1 R01 AG047116-01 09/01/13-06/30/14 $ 441,176
Amyloid β-Protein: Wild Type and Familial Mutant Assembly and Inhibition

NIH General Medical Sciences

Bruce Lipshutz
R01 GM086485 06/01/13-05/31/14 $ 254,335
Transition Metal-Catalyzed Chemistry in Water at Room Temperature

National Institute of Health Subtotal $ 695,511

National Science Foundation

Guenter Ahlers
DMR-1158514 06/01/12-05/31/16 $ 160,000
Turbulent Convection in a Fluid Heated from Below

Dirk Bouwmeester
PHY-1206118 09/01/12-08/31/16 $ 150,000
Quantum Post-Selected Optomechanics

Dirk Bouwmeester
PHY-1314982 09/01/13-08/31/16 $ 90,000
Implementing a Quantum CNOT Gate Using Solid State Cavity QED

Michael Bowers
CHE-1301032 09/01/13-08/31/16 $ 495,000
Peptide Assembly: Mechanism and Inhibition

Mark Sherwin
MCB-1244651 01/01/13-12/31/15 $ 268,910
Robust Gd3+ -Based Spin labels for Structural Studies of Membrane Proteins

Mark Sherwin
DMR-1405964 07/01/14-06/30/17 $ 565,000
Terahertz Electron Hole Recollisions

National Science Foundation Subtotal $ 1,728,910

Novartis Pharmaceutical

Bruce Lipshutz
SB140127 06/15/14-06/15/15 $ 182,000
New Methodologies in Synthesis Using Micelalr Catalysis

Novartis Pharmaceutical Subtotal $ 182,000

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

Douglas Scalapino
4000129396 04/01/14-03/31/16 $ 127,758
Study of the Properties of Strongly Correlated Materials

Oak Ridge National Laboratory Subtotal $ 127,758

Paragon TEC

Jatila van der Veen
SB140043 07/01/2013-08/15/2013 $ 2,500
NASA Summer of Innovation: Planck Mission Education and Outreach

Paragon TEC Subtotal $ 2,500

Raytheon Company

Philip Lubin
SB140137-0001 04/01/14-12/31/14 $ 141,470
Task 1: Advanced Camera Development

Raytheon Company Subtotal $ 141,470

University of Pittsburgh

Mark Sherwin
1468484 07/31/13-07/30/16 $ 346,875
Passively-Cooled, near Quantum Limited Heterodyne Detector for Space Applications including High Resolution Planetary and Cometary Spectroscopy

University of Pittsburgh Subtotal $ 346,875

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

U.S-Israel Binational Science Foundation Subtotal $ 23,515

Research Support Summary
(2013-2014)

		% Total	
Federal			
DAF Office of Scientific Research	7%	7%	240,000
Jet Propulsion Laboratory	3%	3%	92,700
National Institute of Health	22%	19%	695,511
National Science Foundation	53%	48%	1,728,910
Oak Ridge National Laboratory	4%	4%	127,758
Paragon TEC	0%	0%	2,500
University of Pittsburgh	11%	10%	346,875
Federal Totals	100%	90%	$3,234,254

International			
U.S.-Israel Binational Science Foundation	100%	1%	23,515
International Totals	100%	1%	$23,515

Private			
Freedom Photonics	5%	1%	18,388
Novartis Pharmaceutical	53%	5%	182,000
Raytheon Company	41%	4%	141,470
Private Totals	100%	9%	$341,858

Awards Summary

Federal Totals	90%	$3,234,254
International Totals	1%	$23,515
Private Totals	9%	$341,858

TOTALS	**100%**	**$3,599,627**

Charts and Graphs

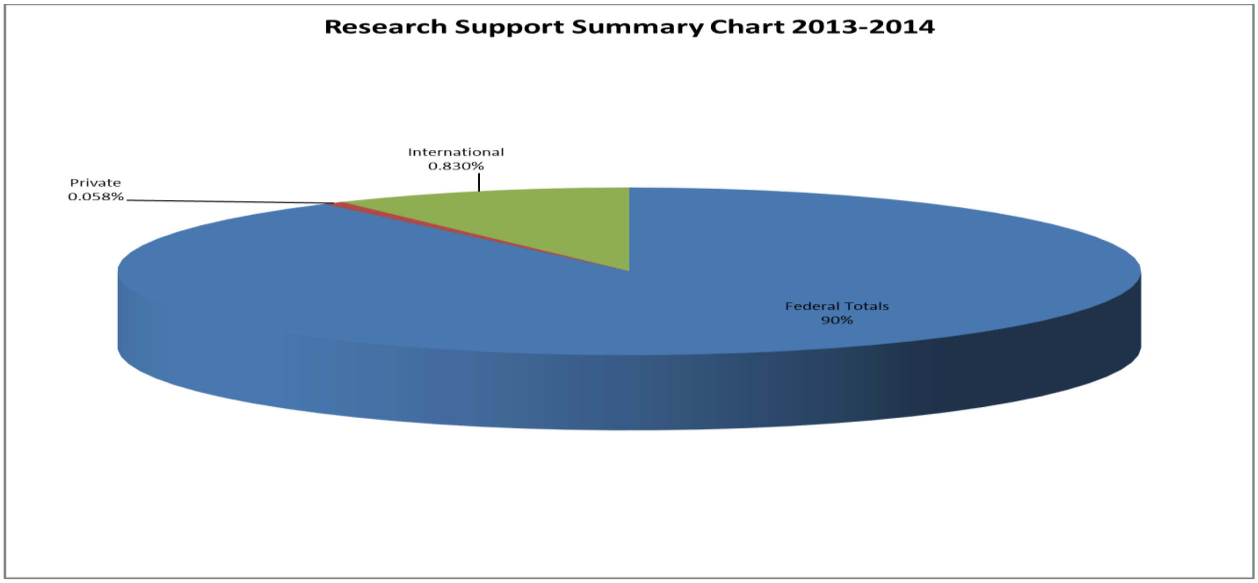


Chart 1: Research Support Summary Chart

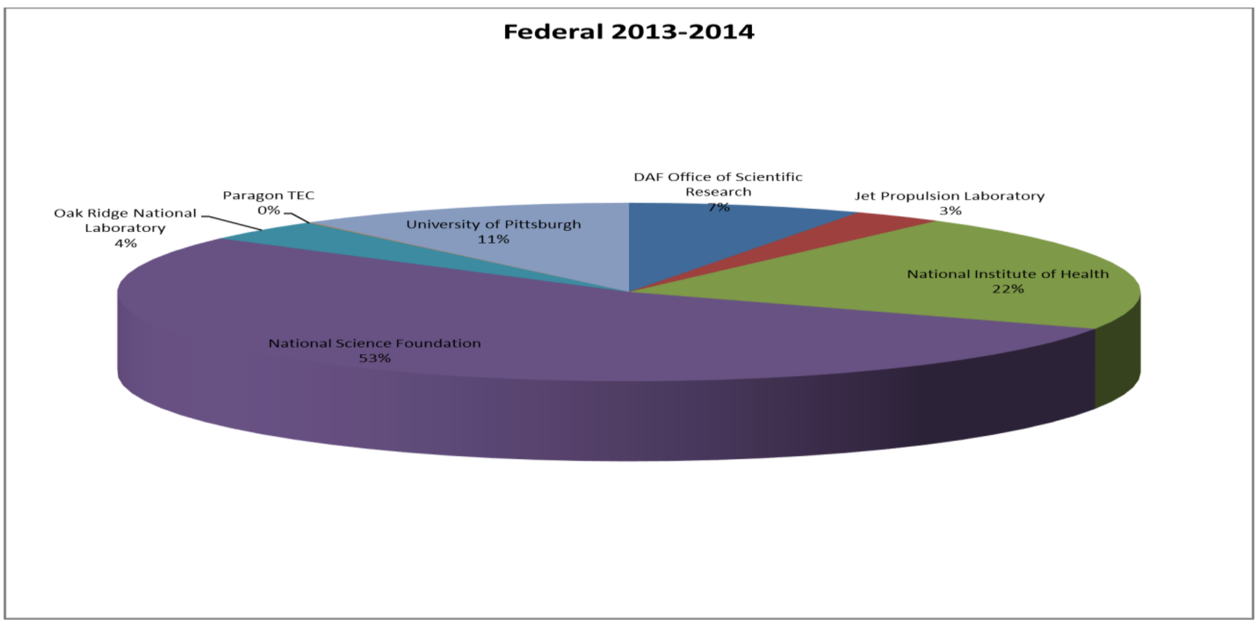


Chart 2: Federal Research Support Summary Chart

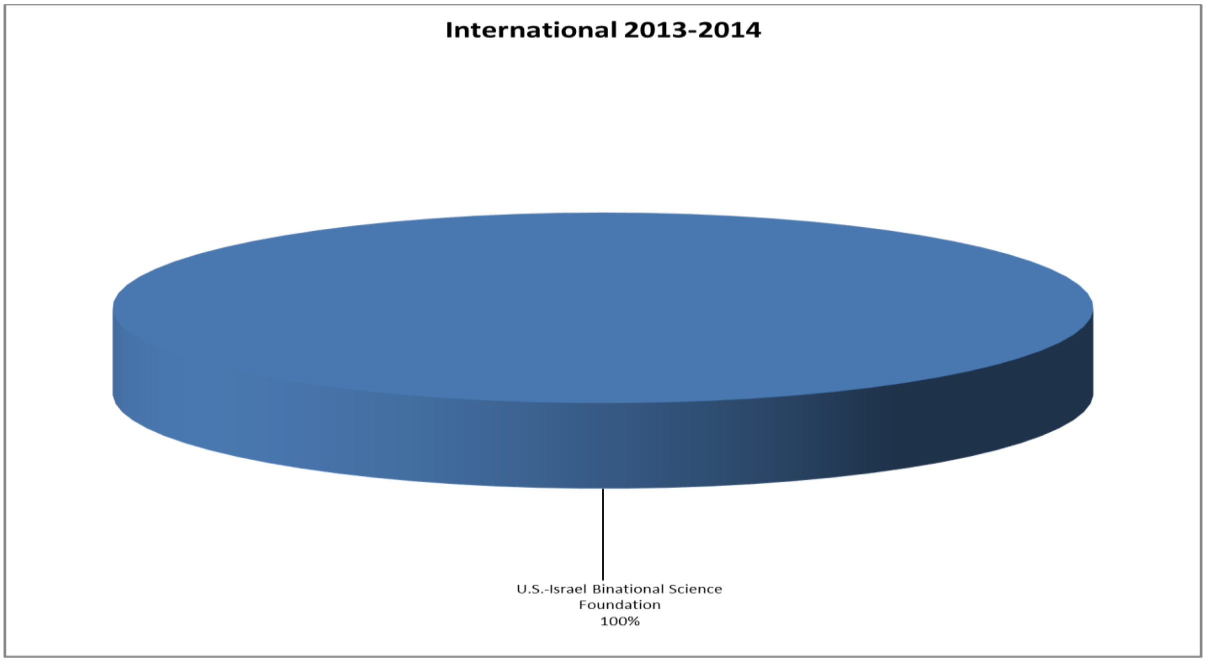


Chart 3: International Research Support Summary Chart

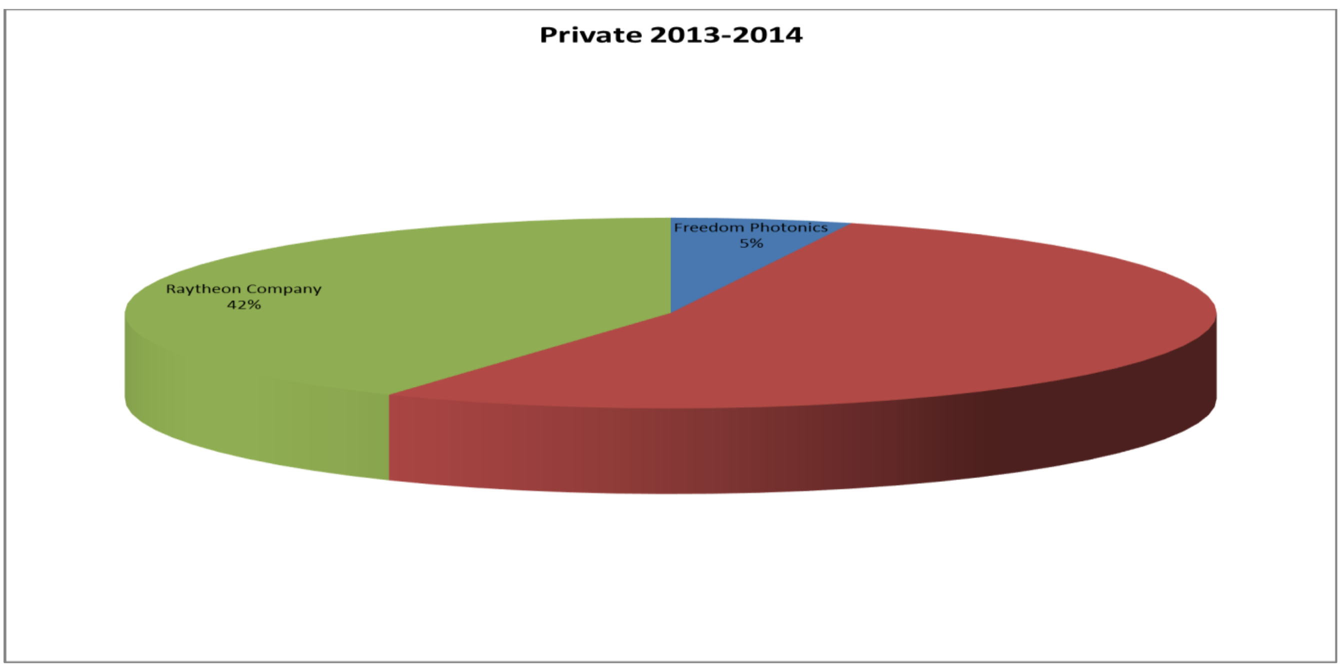


Chart 4: Private Research Support Summary Chart

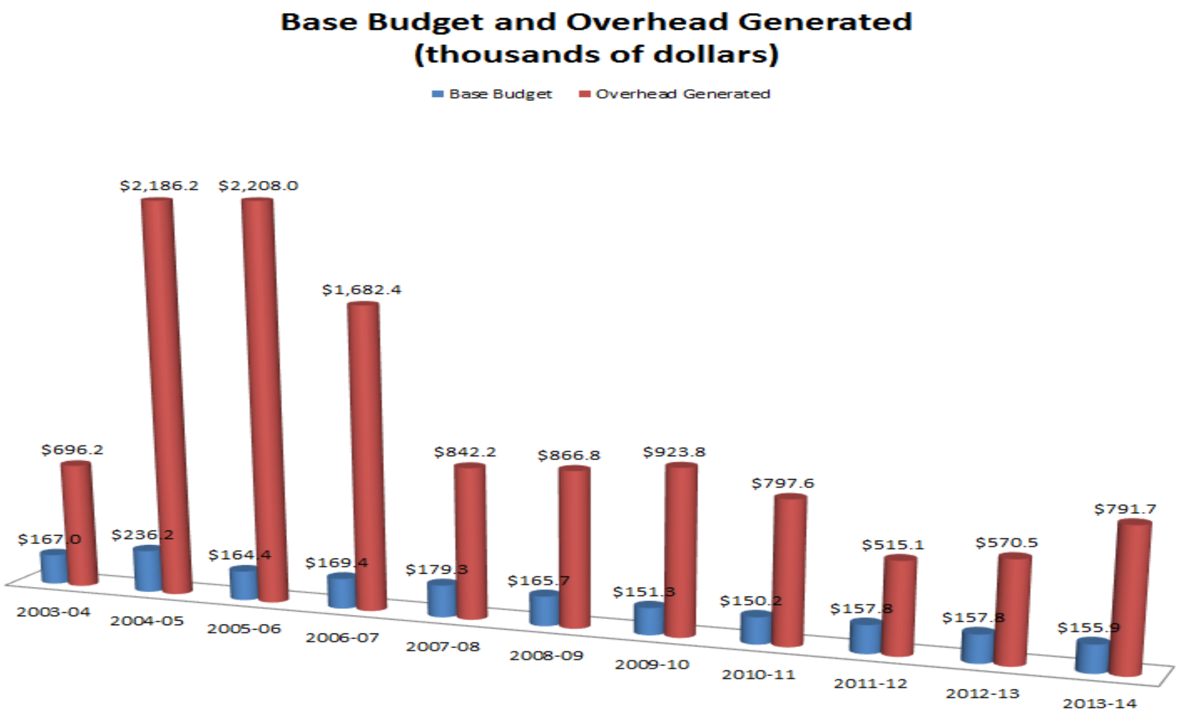


Chart 5: Base Budget and Overhead Generated

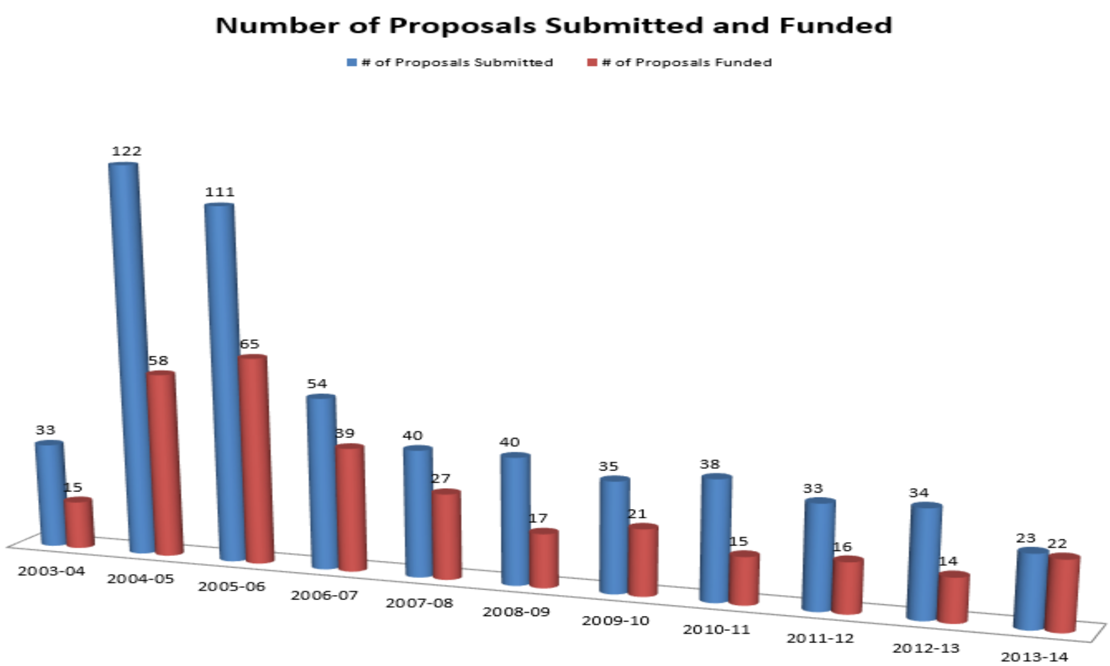


Chart 6: Number of Proposals Submitted and Funded

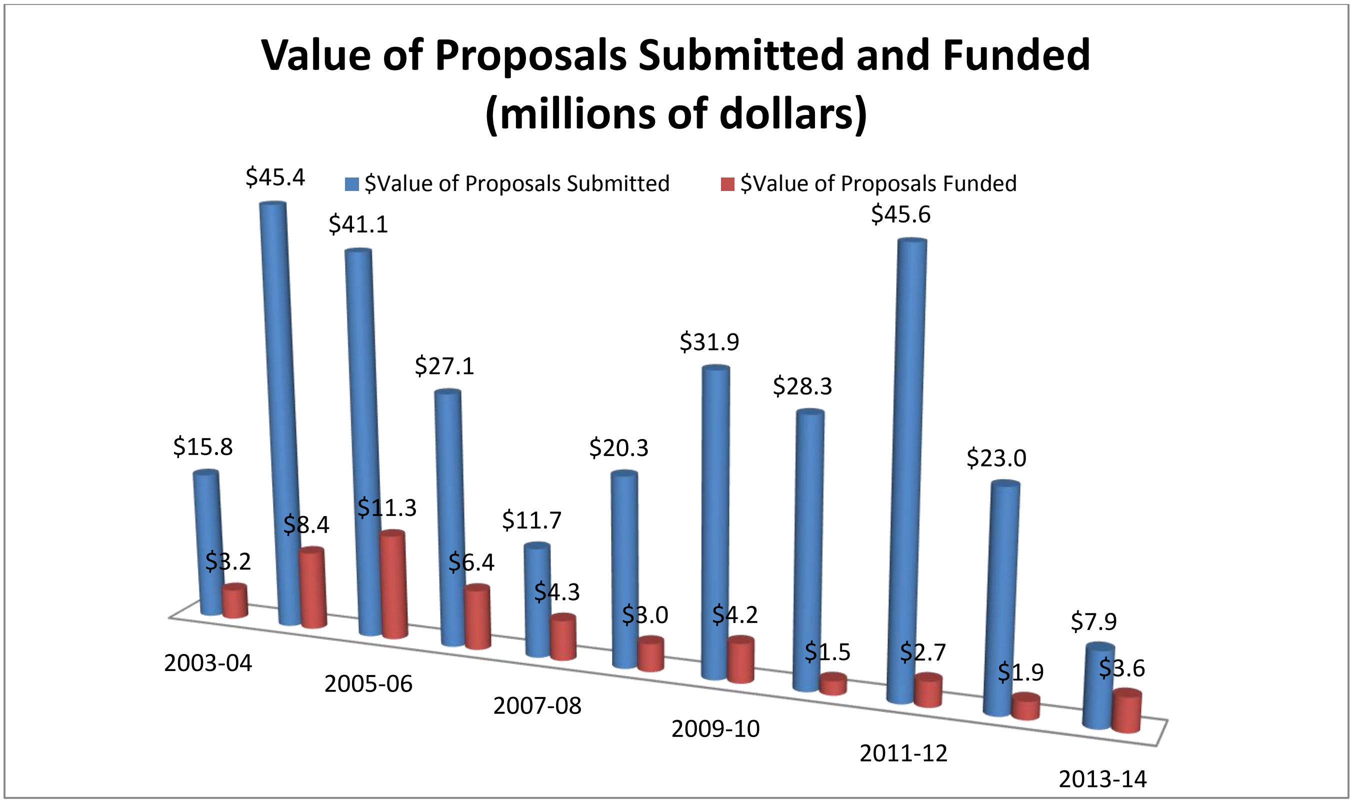


Chart 7: Value of Proposals Submitted and Funded

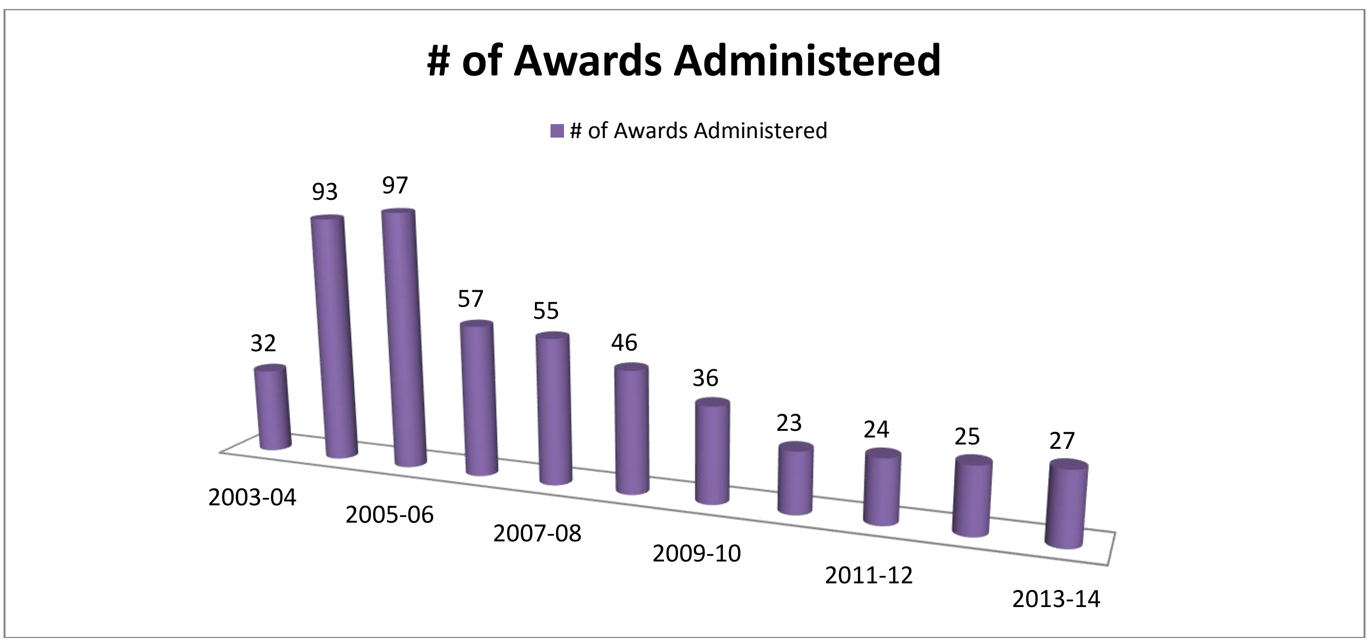


Chart 8: Number of Awards Administered

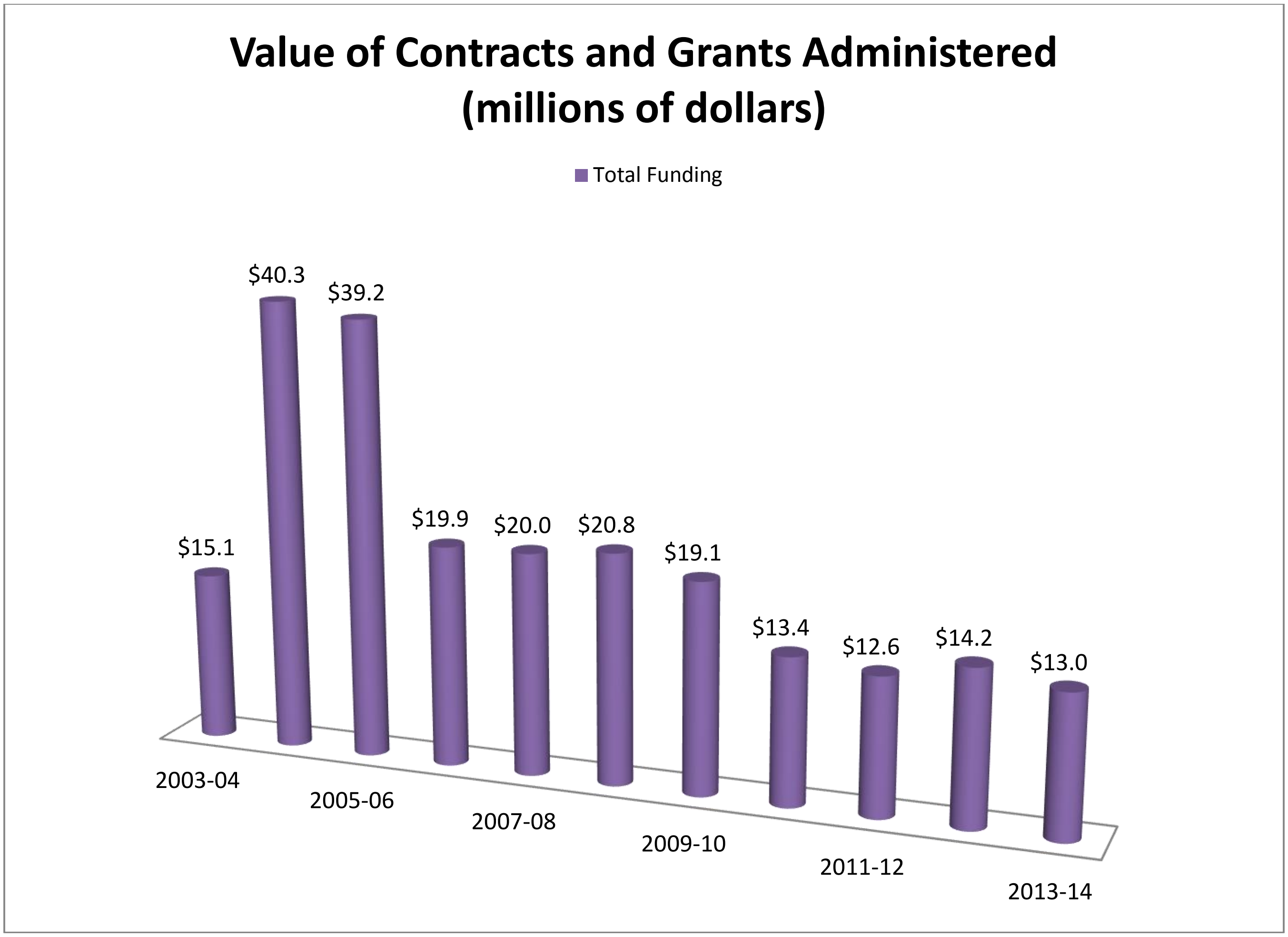


Chart 9: Value of Contracts and Grants Administer

Statistical Summary for ITST

		2013-2014
1. Academic personnel engaged in research:		
a.	Faculty	18
b.	Professional Researchers (including Visiting)	2
c.	Project Scientists	2
d.	Specialists	4
e	Postdoctoral Scholars	4
f	Postgraduate Researchers	
	TOTAL	**30**
2. Graduate Students:		
a	Employed on contracts and grants	30
b.	Employed on other sources of funds	
c.	Participating through assistantships	
d.	Participating through traineeships	
e	Other (specify) Visiting Grad Students	3
	TOTAL	**33**
3. Undergraduate Students:		
a.	Employed on contracts and grants	5
b.	Employed on other funds	
c.	Number of volunteers, & unpaid interns	35
	TOTAL	**40**
4. Participation from outside UCSB: (optional)		
a.	Academics (without Salary Academic Visitors)	6
b.	Other (City College Student)	1
5. Staff (Univ. & Non-Univ. Funds):		
a.	Technical	8
b.	Administrative/Clerical	3
6. Seminars, symposia, workshops sponsored		18
7. Proposals submitted		23
8. Number of different awarding agencies dealt with*		18
9. Number of extramural awards administered		27
10. Dollar value of extramural awards administered during year**		$13,014,996
11. Number of Principal Investigators***		20
12. Dollar value of other project awards ****		$310,682
13. Number of other projects administered		7
14. Total base budget for the year (as of June 30, 2014)		$155,868
15. Dollar value of intramural support		$752,952
16. Total assigned square footage in ORU		7,700
17. Dollar value of awards for year (08 Total)		$3,599,627

* 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	Research Professor	Physics
S. James Allen	Research Professor	Physics
James Blascovich	Professor	Psychological and Brain Sciences
Dirk Bouwmeester	Professor	Physics
Michael Bowers	Professor	Chemistry and Biochemistry
Steven Buratto	Professor	Chemistry and Biochemistry
Deborah Fygenson	Associate Professor	Physics
Elisabeth Gwinn	Professor	Physics
Song-I Han	Professor	Chemistry and Biochemistry
Michael Liebling	Associate 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 Computer Engineering
Douglas Scalapino	Research Professor	Physics
Mark Sherwin	Professor	Physics
Jatila Van Der Veen	Research Associate	Institute for Terahertz Science and Technology/Lecturer College of Creative Studies

Map

Our offices are located at
Bldg 937 west of Broida Hall
PARKING DESIGNATIONS
Permits required at all times.
A Faculty
B1 Residential Students
B2 Residential Students
B3 Residential Students
C Students, Commuters and Visitors
S Staff
R Reserved
V Vendors
Accessible Parking
Motorcycles
Bus Stop
Coastal Access
Residence Halls
Traffic Light
Parking Meters (available to general public)
Parking Dispensers
Parking
Emergency
• For fire, police or medical emergency assistance call 9-911 or use emergency phones (in red boxes).
• UCSB Police Department, Public Safety Building, non-emergency 805-893-3446 (24 hours).
• CSO Escort Service is available by calling 805-893-2000.
SPEED LIMIT 25
UCSB Lagoon