



The Institute for Quantum and Complex Dynamics

U.C. Santa Barbara Home for Terahertz Research

Annual Report 2007-2008

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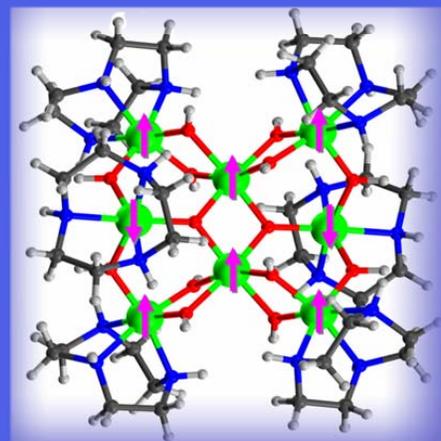


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Mission Statement

The mission of IQCD 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.

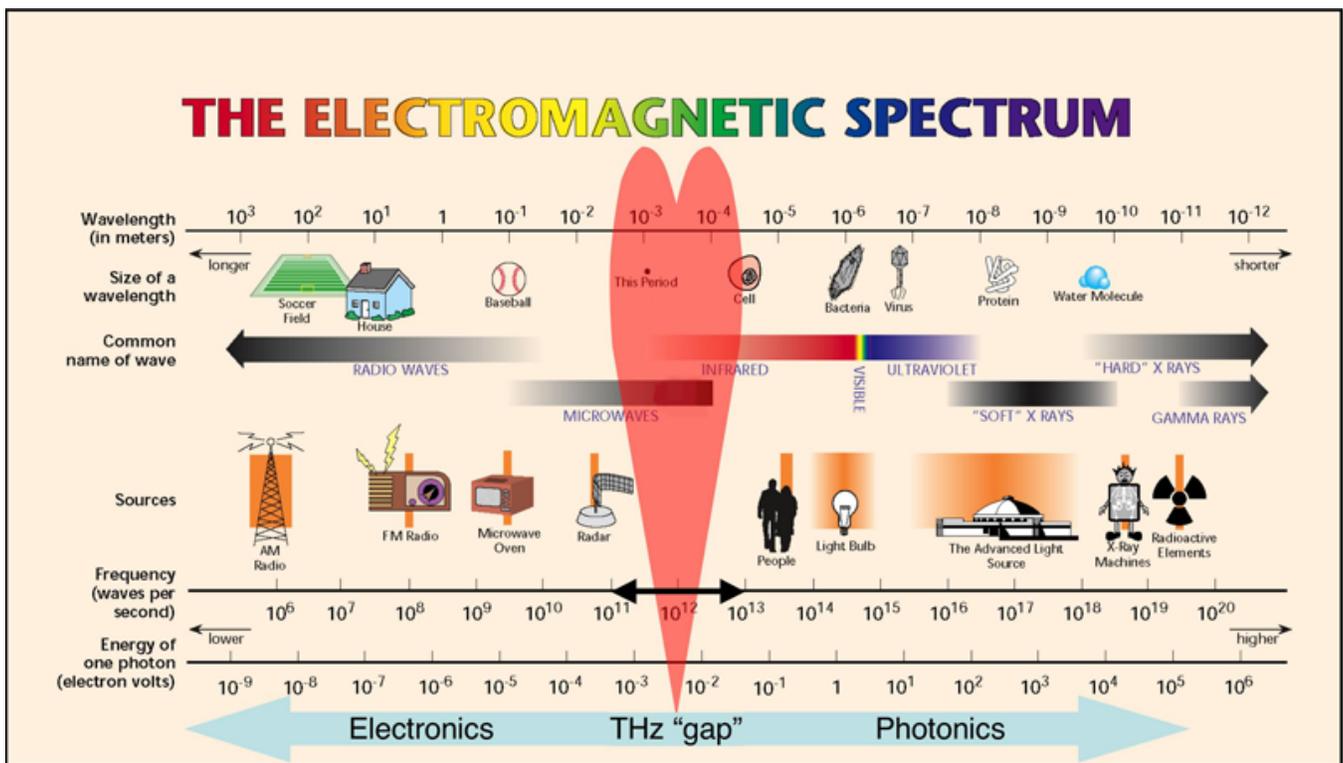


Figure 1: Chart showing IQCD's research emphasis at the heart of the electromagnetic spectrum.

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.

"Electromagnetic spectrum" graphic courtesy of Lawrence Berkeley National Laboratory's Advanced Light Source.

Director's Statement

The intellectual mission of IQCD is “*to advance science and technology at the heart of the electromagnetic spectrum.*” This new intellectual mission statement is one of the results of a year-long strategic planning process that IQCD undertook following the recommendations of our Spring 2007 extramural review. The other two parts of IQCD’s mission statement, a commitment to training, and a dedication to outstanding service, have not changed. I am deeply grateful to all of the members of the IQCD advisory committee, with special thanks to Advisory Committee Chair Prof. Kevin Plaxco, for long hours and intensive consultations that have resulted in a comprehensive three-year strategic plan for the development of IQCD.

As we define it, the “heart of the electromagnetic spectrum,” lies in the neighborhood of one trillion cycles/s, or 1 terahertz (THz). One terahertz is orders of magnitude higher than frequencies accessible to electronic devices like radios, cell phones and radars, but also orders of magnitude lower than the frequency of visible light used in familiar photonic devices like cameras, bar-code scanners and fiber-optic communication systems. Historically, the neighborhood of 1 THz has been a sort of electromagnetic no-man’s land. Now, international research and development in terahertz science and technology are growing explosively. IQCD has a long history of pioneering interdisciplinary research in terahertz science and technology, anchored by but not limited to our unique Free-Electron Lasers. UCSB has tremendous strength in terahertz research with renowned faculty in the Departments of Physics, Mathematics, Chemistry and Biochemistry, Electrical and Computer Engineering, and Materials.

IQCD is the home UCSB needs for interdisciplinary research in terahertz science and technology. Research at terahertz frequencies requires expensive, exotic apparatus and rapidly-evolving techniques which present a high barrier to those who would simply like to use terahertz technology. Terahertz technology has been applied to disciplines ranging from art history (researchers at UC San Diego are beginning to use terahertz spectroscopy to look through surface layers of famous works of art to see the underdrawing) to molecular biology. IQCD’s strategic plan calls for enhancing its impact on and off campus by maintaining state-of-the-art capabilities for terahertz research while reaching out to researchers who may find these tools and expertise useful, regardless of discipline.

Heralding a new and highly interdisciplinary direction, IQCD this year received a major W. M. Keck Foundation Science and Engineering Grant entitled “*‘Filming’ proteins in action with the UC Santa Barbara Free-Electron Lasers.*” With this award, IQCD is pushing the powerful technique of electron spin resonance to high enough frequencies and powers that it will be able to resolve the rapid motions of proteins as they perform their biological functions. IQCD is also acquiring two state-of-the-art spectrometers which complement each other and the UCSB Free-Electron Lasers. These spectrometers will enable a wide range of new interdisciplinary research projects.

This year, a major result in the area of quantum information processing was achieved using electron spin resonance at 0.24 THz. Electron spins localized at sparse sites in diamonds are a very promising potential quantum bit. One of the most important figures of merit for a quantum bit is the decoherence time, the length of time it can exist in one of its quantum states before being significantly perturbed by the environment. Takahashi and co-authors showed that the dominant decoherence mechanism was interactions with a “bath” of other spins in the diamond, and that this decoherence mechanism could be completely quenched by cooling the spin bath to low temperatures.

IQCD looks forward to an exciting year of building up new capabilities and interdisciplinary collaborations while implementing our strategic plan to enhance our impact at UCSB and beyond.

Center for Terahertz Science and Technology

The Center for Terahertz Science and Technology was founded by Prof. Jim Allen and has been in existence for more than 15 years. This Center forms a strong foundation for the strategic plan for all of IQCD.

The faculty at UCSB who are already involved in terahertz research include

- S. James Allen (Physics)
- Elliott R. Brown (Electrical and Computer Engineering (ECE))
- Andrew N. Cleland (Physics)
- Arthur C. Gossard (Materials)
- Songi Han (Dept. of Chemistry and Biochemistry (DCB))
- Philip M. Lubin (Physics)
- Pierre M. Petroff (Materials)
- Kevin W. Plaxco (DCB)
- Mark Rodwell (ECE)
- Mark S. Sherwin (Physics)

External collaborators working with the Center include

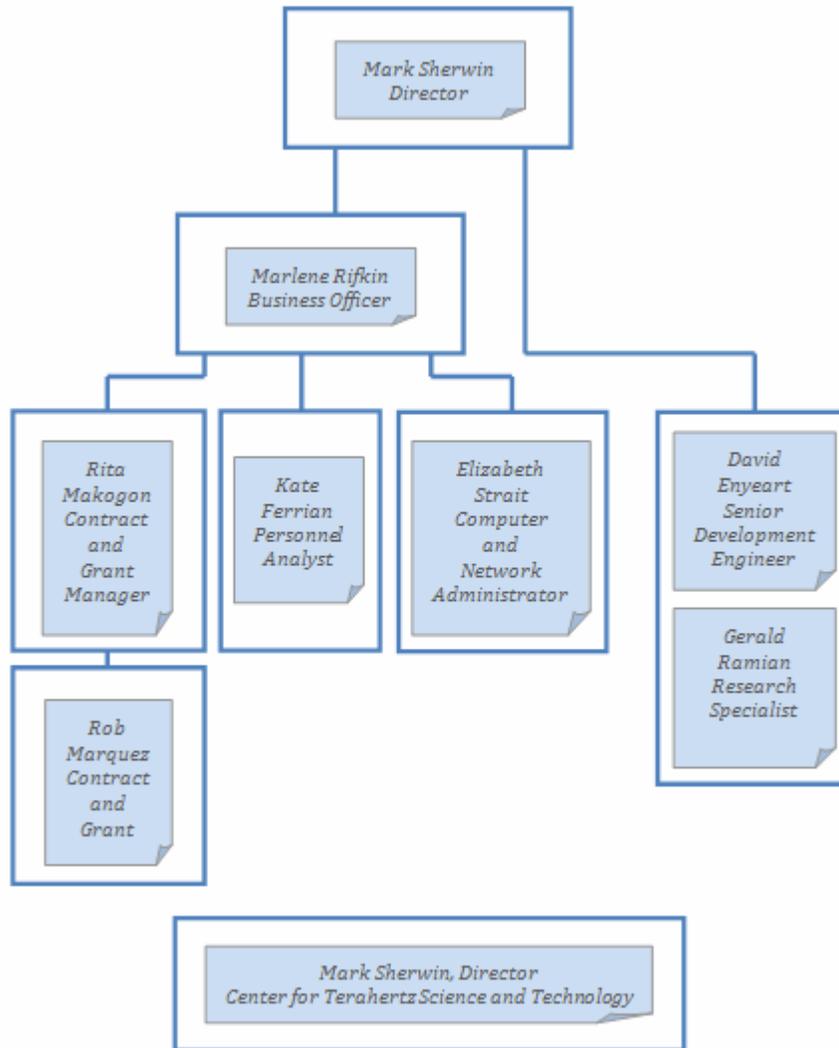
- Hans van Tol (National High Magnetic Field Laboratory (NHMFL), Tallahassee, FL)
- Louis-Claude Brunel (NHMFL), moved to UCSB October 2008
- Zafar Iqbal (Chemistry and Environmental Sciences, New Jersey Institute of Technology)
- Michael Wanke (Sandia National Labs)
- Eric Shaner (Sandia)

On the Keck award, Allen, Brown, Han, Lubin, Plaxco, Rodwell and Sherwin from UCSB were joined by van Tol and Brunel from the NHMFL, illustrating the interdisciplinary breadth of terahertz research on this campus.

New capabilities developed over the past year include electron spin resonance (ESR) at 0.24 THz (magnetic field of 8.5 T). Electron spin resonance is an extremely powerful tool widely used in chemistry, physics and materials science. Usually, ESR is carried out near 10 GHz (0.01 THz). The advantages of going to much higher frequencies include increased sensitivity, spectral resolution, time resolution, and the ability to completely quench thermal fluctuations of the spins.

Community-building activities included lunchtime seminars (with pizza) by external speakers. The seminar series was sporadic last year, but this year we are making it a weekly event and liberally mixing seminars by students and post-docs with seminars by outside speakers. The seminars are on Thursdays at 12:30 pm in 3302 Broida Hall, and we welcome anyone to drop by!

Organizational Chart



Advisory Committee

Kevin Plaxco **Chemistry & Biochemistry, Committee Chair**

| | |
|--------------------|---|
| S. James Allen | Former iQuest Director, Physics |
| Elliot Brown | Electrical and Computer Engineering |
| Frank Doyle | Chemical Engineering |
| Art Gossard | Materials and Electrical and Computer Engineering |
| Songi Han | Chemistry and Biochemistry |
| Michael C. Martin | Lawrence Berkeley National Laboratory |
| Joan-Emma Shea | Chemistry and Biochemistry |
| David Stuart | Physics |
| Chris Van de Walle | Materials |

Ex Officio Members

| | |
|----------------|--|
| Marlene Rifkin | Business Officer, iQCD |
| Mark Sherwin | Director, iQCD, Center for Terahertz Science and Technology, Physics |
| Mark Srednicki | Chair, Physics |

Personnel

Administrative Staff-iQCD

| | |
|-----------------|----------------------------|
| Marlene Rifkin, | Business Officer |
| Kate Ferrian | Personnel Analyst |
| Rita Makogon | Contract and Grant Manager |
| Rob Marquez | Contract and Grant Analyst |
| Keo Xiong | Student Assistant |

Technical Staff-iQCD

| | |
|------------------|------------------------------------|
| David Enyeart | Senior Development Engineer |
| Gerald Ramian | Research Specialist |
| Elizabeth Strait | Computer and Network Administrator |

Other Project and Activities

Seminars and Workshops

This year IQCD hosted a 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.

- 09/26/07:** Dong Kwon Kim, Georgia Institute of Technology.
Optimization of Quantum-Well Electroabsorption Modulators

- 01/24/08:** Benjamin Williams, UCLA
Terahertz Quantum Cascade Lasers

- 02/14/08:** Brian Patton, Princeton University
Spin-Exchange Optical Pumping of Solids

- 03/18/08:** Daniel Mittleman, Rice University
Terahertz Spectroscopy in the Near Field

- 05/02/08:** Gernot Fasching, Vienna University of Technology
Microcavity Quantum-Cascade Lasers: Confinement and Coupling in the
Terahertz Spectral Range

Outreach Program

The Questboards outreach program teaches elementary school students the basics of circuits, electricity, and magnetism. The Questboards are plastic boards with basic circuit elements on them, which students can connect together to create complete electrical circuits. Structured material is given out along with the Questboards to guide the student, and they are also given opportunities to explore the boards on their own.



Figure 2: Our outreach program serves the children in our local community

The Questboards program has been very successful in the past year. In the summer of 2007, two undergraduates helped design and construct two new models of Questboards. A classroom set of 30 of each board was constructed. These boards were designed to teach the concepts of electricity and magnetism required by the California fourth grade state standards. A science specialist from the Goleta Union School District wrote educational material and activities to go along with each of the boards. During the last school year the Questboards have been used in a number of classrooms and at school wide science nights throughout the Santa Barbara area. Over 500 students used the new Questboards at these events. In addition, 15 fourth grade teachers in the Science Matters program in the Carpinteria School District went through a day long Questboards training session and have used them in their classrooms throughout the year with great success. In the next school year we hope to increase the use of the boards in individual classrooms through the teacher contacts we have made this year at various schools in the area, as well as continue the current classroom science night use of the Questboards.

Published Doctoral Dissertations

Dan Allen: *Optical detection of quantum dynamics in GaAs neutral donors*

Dena Bodzin: *Structural characterizations of two systems using ion mobility mass spectrometry: fluoridated polyhedral oligomeric sissequioxanes and a critical segment of the tau protein*: 2008

Eric Brown: *Heat transport and dynamics of the large-scale circulation of turbulent Rayleigh-Bénard convection*: 2007

Huang Yaodong: *Synthesis of brazilin and the core of an ornate scyphostatin analog*: 2007

Young Sam Park: *Housane radical cation chemistry and its application to natural product synthesis using indirect electrolysis*: 2008

Tue Petersen: *Control of atropisomerism en route to the michellamines: Aqueous Suzuki-Miyaura couplings at ambient temperatures. Studies in asymmetric CuH chemistry* : 2008

Stephanie Sohn: *N-heterocyclic carbene catalyzed redox reactions*: 2007

Virginia Tanis: *Studies toward an SAR understanding of the anti-inflammatory/wound healing activity of simplified seco-pseudopterosins and Titanium (III) – mediated formation of C-glycosides: a continuation of the Little/Parrish Study*: 2007

Xiaohua Zhang: *Computational study of enzyme activity and binding affinity*: 2007

Awards Administered

(July 2007 – June 2008)

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

Guenter Ahlers

National Aeronautics and Space Administration, NAG3-2872

Boundary Effects on Transport Properties and Dynamic Finite-Size Scaling Near the Superfluid-Transition Line of ^4He

03/26/03-09/30/07

\$614,000

We extended the analysis of the thermal conductivity measurements of helium confined in cylindrical channels of glass capillary arrays to the case of rectangular channels. Measurements were made on plates with channels of 1x10 micro-m cross section, and simultaneously on bulk helium. To our great surprise the results show that the finite-size scaling-function for this geometry does not differ measurably from the scaling function for cylindrical confinement. This differs qualitatively from what had been found for thermodynamic properties in one-dimensional and two-dimensional confinement. We have now started the measurements of the heat capacity in the same micro-channel plates. Knowledge of this is necessary for the complete theoretical interpretation of the conductivity data. Results have been obtained for cylindrical channels of diameter 1 micro-m.

Guenter Ahlers

National Science Foundation, DMR-0243336

Stochastic Effects in Systems Far From Equilibrium

05/01/03-04/30/08

\$620,000

This work focuses on quantitative studies of fluctuations caused by thermal noise below and near bifurcations in systems far from equilibrium. Well below the bifurcation it is expected that the measurements will test recent predictions about the structure factor of a fluid in a thermal gradient. Near the bifurcation the nonlinear interactions between the fluctuations should lead to critical phenomena in the sense that the various measurable quantities will deviate non-trivially from mean-field (or linear) predictions. The experiments will focus on Rayleigh-Bernard convection (RBC) in a horizontal layer of a fluid heated from below, and on electro convection (EC) of a nematic liquid crystal in an electric field. It has been predicted that RBC belongs to a universality class first studied theoretically by Brazovskii for which fluctuations change the bifurcation from a second-order to a first-order transition. For electro

convection there is at present no theory of the critical behavior, but on general grounds one expects several different universality classes that depend on the relationship between the nematic director and the convection-roll wave director. The experiments will open a new research field of critical phenomena in non-equilibrium systems, and will prepare graduate students and postgraduate researchers for academic or industrial careers. Within an outreach program they will offer opportunities for participation by high school students. Many properties of equilibrium systems exhibit large thermally driven fluctuations near critical points. An example is the density of a fluid near a liquid-gas critical point. Nonlinear interactions between the fluctuations then cause the critical behavior to be different from that which is expected when fluctuations are small. The same phenomena should occur in a very different context, namely near transitions in non-equilibrium systems. For example, the transition from pure conduction to convection in a thin horizontal layer of a fluid heated from below was predicted to be of second order when fluctuations were neglected, but to become a first-order transition when they were considered. This work will determine the critical behavior near transitions in several non-equilibrium systems, including convection in a fluid heated from below and convection in a liquid crystal exposed to an electric voltage. This research will use advanced experimental techniques and sophisticated numerical image analysis, which will provide excellent training of graduate students for careers in academic and industrial positions. It also lends itself well to the participation of undergraduate students. Within an outreach program it is expected that high school students will also participate in some of the experiments.

Guenter Ahlers

Department of Energy, DE-FG02-03ER46080

Heat Transport by Turbulent Rayleigh-Benard Convection

09/15/03-3/13/08

\$574,226

This award focuses on the study of turbulent Rayleigh-Benard convection. Turbulent convection is of fundamental interest in nonlinear science, relevant to practical problems involving energy transport in fluid flow, and a significant ingredient of natural phenomena in the Earth's atmosphere and oceans as well as in the stars. In addition to providing data needed to verify recently developed theoretical models of turbulent convection, our results will contribute to the elucidation of seemingly conflicting results obtained in experiments by others at very large Rayleigh numbers.

Guenter Ahlers

National Science Foundation, DMR-0702111

Turbulent Convection in a Fluid Heater from Below

05/01/07-04/30/09 (04/30/12)

\$310,000 (\$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

13

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

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)

06/15/06-02/28/09 (06/14/09)

\$484,216 (\$681,665)

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

\$579,045

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 -dihydroamino 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

American Chemical Society, PRF 43246-G1

Development and Applications of New Reactions for Chemoselective Amidations

09/01/05-08/31/07

\$35,000

Detailed studies and applications of a new approach to direct, chemoselective amidation by decarboxylative condensations of hydroxylamines and α -ketoacids are proposed. This novel process proceeds in polar solvents (DMF, DMSO, H₂O) under mild reaction conditions and displays remarkable functional group tolerance. On the basis of our preliminary findings we will pursue the development and mechanistic understanding of this unique process. These studies will lead to innovations in substrate scope, including the use of cyclic hydroxylamines amines as substrates for an iterative, waste-free approach to the iterative synthesis of poly- β -peptides. In addition, we will utilize these new reactions for preliminary studies towards the facile polymerization of hydroxylamine amine monomers.

Jeffrey Bode

Research Corporation, CS1392

New Ligation Reactions for the Synthesis of Biomolecules and Biomaterials

07/01/06-06/30/09

\$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- β -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 peptodomimetics. 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, peptodomimetics, and biocompatible materials.

Jeffrey Bode
Arnold and Mabel Beckman Foundation, SB060113
Chemical Peptide Synthesis without Reagents, Protecting Groups, or By-Products
09/01/06-10/11/07
\$264,000

The chemical synthesis of polypeptides is limited to the preparation of relatively small amounts of relatively short sequences through procedures that are often expensive and inefficient. Furthermore, the constraints of protecting groups, scale, and cost inherent to traditional peptide synthesis impede the synthesis of proteins, glycopeptides, polypeptide-based biomaterials, and polypeptide biomimetics such as peptide nucleic acids (PNA) and poly- β -peptides. To address these limitations, we have recently developed a mechanistically unique approach to polypeptide synthesis that does not require coupling reagents or protecting groups and produces carbon dioxide as the only by-product. Based on this novel process, we will pursue 1) chemical ligation strategies to synthesize proteins and glycopeptides, 2) new approaches to iterative and templated polypeptide synthesis, and 3) the preparation of functionalized β -peptides by living polymerizations in water.

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

\$30,913

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.

Jeffrey Bode

David and Lucille Packard Foundation, 2006-30522

New Chemical Ligation Reactions for Biomolecular Synthesis and Engineering

10/20/06-09/30/07

\$59,529

By developing a new generation of chemical reactions that will greatly expand the possibilities of biomolecular synthesis and engineering, Dr. Jeffrey Bode is redrawing the boundaries between synthetic organic chemistry and molecular biology. He has developed an unprecedented process for creating amide bonds, the key chemical connection in all living things, without the need for reagents or masking groups and without producing the usual toxic by-products. This novel chemical ligation has the potential to transform the synthesis of modified proteins, thereby opening new avenues to the production of new therapeutic agents and models for the understanding and treatment of disease. Furthermore, his work offers the first method for the synthesis of stable, biocompatible materials under physiological conditions with far-reaching applications in tissue engineering, scaffolds for stem-cell production, and polymer synthesis in vivo.

Jeffrey Bode
Biomeasure Incorporated, SB070066
Ligation Strategies for Peptide Synthesis and Modification
01/01/07-11/16/07
\$134,632

This research seeks to achieve two specific goals: 1) The chemical synthesis of glucagon-like peptide 1 (GLP-1) amide (7-36) via ketoacid-hydroxylamine peptide ligations and 2) the development of new ligation methods for the post-synthetic modification of peptides.

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 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 as high-school students participating in the UCSB summer science education program.

Dirk Bouwmeester

National Science Foundation, PHY-0804177

Quantum States of OptoMechanical Structures

05/03/08-07/31/09 (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 Schrodinger'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 Antermortem Test for Bovine Spongiform Encephalopathy: An Ion Mobility/Mass Spectrometry Approach

01/01/05-12/30/07

\$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

Air Force, FA9550-05-1-0280

Ultra High Resolution Ion Mobility Instrument

04/01/05-03/31/07

\$352,235

A request is made for an ultra high resolution ion mobility machine that will greatly increase our ability to resolve both conformers and geometric isomers of complex systems. In recent years we have frequently encountered systems where we have been unable to resolve structural isomers and thus could not provide accurate feedback to synthetic groups we are collaborating with. We are convinced that this will become a much more serious issue as we intensify our collaborations with the POSS synthesis group at Edwards AFB. A second application for the new machine involves size-elected metal clusters where structural isomers are common but cross sectional differences are often small. Being able to accurately determine structural identities of these clusters and obtain structurally resolved energetic and reaction information will greatly assist the ongoing effort in catalysis research funded under a DURINT grant. The instrument will take advantage of known technology but with improvements we hope will increase sensitivity by up to a factor of 10. Current instrumentation is limited to a resolving power of $\Delta t/t \approx 20$ at room temperature while the new machine will routinely provide a resolving power of at least 180. When cooled to liquid nitrogen temperatures, resolutions of ~ 300 are expected.

Michael Bowers

National Science Foundation, CHE-0503728

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

07/01/05-04/30/08

\$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

01/01/06-11/30/07 (11/30/08)

\$369,000 (\$558,000)

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.

Thomas C. Bruice

Public Health Service/National Institutes for Health, R37 DK09171

Biomechanical Mechanisms-Enzymes, Cancer and Models

09/01/02-08/31/07

\$2,644,059

The major goals of this project fall into three categories: (i) blocking of the binding of certain protein transcription factors (TF) to their consensus DNA binding sites, (ii) specific inhibition of DNA and RNA function (antisense and antigene agents), and (iii) understanding the structural basis for RNA self splicing.

Steven Buratto

Michael Bowers

Department of Energy/Miscellaneous Offices and Programs, DE-FG02-06ER15835

Chemical Imaging with 100nm Spatial Resolution

09/01/06-08/31/07 (08/31/09)

\$262,188 (\$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 LSCM 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

04/01/08-03/31/09 (03/31/10)

\$202,000 (\$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 and Ag mass-selected clusters supported on oxide, (b) very small mass-selected, binary clusters such as PdAu 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

\$65,000 (\$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
07/01/06-06/30/09
\$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
03/01/04-06/30/08
\$1,094,820

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 Daugherty
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
08/01/06-07/31/08
\$2,000,000

Purchase of an 800 MHz NMR Spectrometer.

Peter Ford
Susannah Scott
University of Washington, 919941
Time-Resolved Spectroscopy on Dehydrogenation Systems
09/01/04-08/31/07
\$151,792

This research is concerned with utilizing flash photolysis techniques to generate reactive intermediates from various iridium pincer complexes prepared at the University of Washington. Time resolved optical (UV/vis) and infrared detection will be used to accumulate the TRO and TRIR spectra of these intermediates and to identify the products subsequently formed. The quantitative effects of variations of the media and other reaction conditions on the decay dynamics of these intermediates and upon their eventual products will allow one to define what roles these species might play in alkane dehydrogenation and other catalytic pathways of these iridium complexes.

Deborah Fygenon
Dirk Bouwmeester
National Science Foundation, CCF-062257
DNA Patterned Pairs of Colloidal Quantum Dots: A Scalable Approach to Computing Without Wires
09/01/06-08/31/08 (08/31/09)
\$200,000 (\$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 a powerful new class of self-assembling DNA scaffolds that can template arbitrary complex patterns with 6 nm resolution.

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 endiayne.

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****02/01/06-01/31/09 (01/31/10)****\$444,000 (\$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.

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 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 (\$120,000)

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

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

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.

Horia Metiu

Michael Bowers

Steven Buratto

Martin Moskovitz

Eric McFarland

Air Force, F49620-01-1-0459

Catalysis by Nanostructures: Methane, Ethylene Oxide, and Propylene Oxide

Synthesis on Ag, Cu or Au Nanoclusters

07/01/01-08/31/07

\$4,519,452

UC Participation: \$120,012

We study, theoretically and experimentally, catalysis by small supported metallic clusters. Our calculations have determined the binding of Au, Ag, H₂ and O₂ to Au clusters, TiO₂ and Au/TiO₂. We have built an instrument that prepares mass-selected clusters, deposits them on a surface and examines their properties by STM and surface science methods. We have discovered that K salts promote CO oxidation by Au/TiO₂. We demonstrated that electric fields applied across the surface of an oxide catalyst can modify its catalytic properties.

Thomas Pettus

Public Health Service, National Institutes of Health, GM64831

The Synthesis and Application of Chiral Cyclohexadienones

01/01/02-12/31/07

\$1,295,154

Small cell-permeable natural products and their analogs play a crucial role in the treatment of disease. This grant addresses the syntheses of several biologically active molecules relevant to the treatment of cancer, HIV, stroke and heart disease through optically enriched chiral cyclohexadienones that until now have been relatively inaccessible chemical entities. Their fragile nature coupled with the lack of enantioselective access has hampered their widespread synthetic applications. The Pettus group has shown that robust enantiopure cyclohexadienones can be constructed to undergo a myriad of diastereoselective reactions including 1,2-, 1,4- and 1,6-additions, along with various rearrangements and cycloadditions. Telomerase, an enzyme responsible for telomere elongation, has been recently linked to the immortalization of cells and cancer. Most somatic cells, with the exception of rapidly

regenerating tissue such as bone marrow, show little to no telomerase activity. However, 85%-90% of human breast cancer cell lines demonstrate upregulated telomerase activity. It has been suggested that telomerase holds the key to cancer cell immortality. Therefore, by inhibiting telomerase, it should be possible to prevent cancer cells from dividing indefinitely, leading to eventual tumor death with minimal side effects. One such telomerase inhibitor of unknown stereochemistry, diazaphilonic acid, was recently discovered. The Pettus group is pursuing a synthesis of diazaphilonic acid.

Norbert Reich

UC Discovery Grant-Biotechnology, bio05-10524

Tamarisc Diagnostics, SB060120

Rapid Detection of HPV in Clinical Samples

04/25/06-04/24/08

\$81,267

Human Papillomavirus (HPV) infection in the human population can lead to cancer and there is an immediate need for robust, inexpensive, and rapid diagnostics to detect HPV, both in and out of the clinic. We will develop a technology to be incorporated into a point of care diagnostic which enables the rapid and accurate detection of HPV. Our goal is to carry out viral typing to further facilitate treatment of the high risk HPV types associated with cancer. The detection is based on a simple and robust optical principle involving fluorescently labeled molecules, which only emit light in the presence of the viral genome. Currently, we are able to detect as little as 100 fmoles of a target DNA sequence with high precision, at a cost of under \$3 per assay. Our goal is to optimize an assay that will be accurate, economic, efficient, and can be performed by non-specialists for broad application.

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
S. James Allen
David Awschalom
Daniel Blumenthal
Pierre Petroff
Kevin Plaxco
Jerry Ramian

National Science Foundation, DMR-0321365

**Development of a Stable, User-Friendly, High-Power Terahertz Source:
Enhancements to the UCSB Free-Electron Laser**

08/15/03-07/31/07

\$425,000

UC Participation: \$96,000

The UCSB Free-Electron Lasers and newly-renovated User's Lab stand out as unique facilities which enable measurements that can be done nowhere else. The FELs work as follows. An electrostatic accelerator generates a beam of electrons with energies ranging from 2 to 6 MeV. The electrons are injected into one of two fully operational free-electron lasers before being recirculated. Narrow-band light emitted by the relativistic free-electron beam as it moves through the undulators in these lasers is amplified and trapped in a resonator. The small fraction which is coupled out is typically 1kW, tunable from 140 GHz to 5 THz, with pulse durations of a few μ s.

The three enhancements undertaken are: 1. Modernize control system 2. Stabilize frequency 3. Build a FEL spectrometer.

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-

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
07/11/06-07/10/07
\$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
07/01/07-06/30/09 (06/30/10)
\$260,000 (\$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.

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.

Petra Van Koppen

Camille & Henry Dreyfus Foundation, SG-05-081

Outreach Program to Improve Educational Opportunities for K-12 Students: A Hands-on Inquiry-Based Approach to Teaching Physical Science in the Fifth Grade

01/01/05-12/31/07

\$24,661

UC Participation: \$9,974

Outreach Program Goals:

- **Physical science summer workshop for elementary school teachers**
 - Provide standards-based content and activities for fourth and fifth grade teachers
 - Give teachers the opportunity to design and present activities
 - Provide ready to use classroom lessons
 - Provide hands-on activities and applications to real world problems and everyday experiences
 - Enable teachers to apply learned skills in their classroom: prepare their students to participate in a chemistry outreach workshop at UCSB

 - **Chemistry outreach program for fifth grade students, parents and teachers**
 - Enable students from diverse backgrounds to work with UCSB students who are also from diverse backgrounds
 - Spark new interests in sciences and fuel current interests
 - Show students the relevance of chemistry
 - Engage students, parents and teachers in exciting hands-on activities
 - Enable volunteers to share their enthusiasm for science with young students
 - Inspire students to pursue a higher education in science
 - Show elementary school students the excitement of working in a college setting
-

Contracts/Grants Awarded 2007-2008

Air Force

Michael Bowers
FA9550-06-1-0069 01/01/06-11/30/08 \$ 189,000
POSS and Metal Clusters: Structures and Energetics

Army

S. James Allen, Kevin Plaxco
W911NF-06-1-0241 06/15/06-02/28/09 \$ 224,470
Sloan Research Fellowship

Department of Energy

Steven Buratto, Michael Bowers
DE-FG02-06ER15835 09/01/07-08/31/08 \$ 165,375
Chemical Imaging with 100nm Spatial Resolution

Environmental Protection Agency

Galen Stucky
SB060043 09/01/05-08/31/08 \$ 15,007
US EPA Fellowship

Florida State University

Mark Sherwin
R00501 11/01/05-08/31/08 \$ 31,014
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

Jet Propulsion Laboratory

Philip Lubin
JPL 1289807 09/21/06-09/30/08 \$ 17,500
Planck Educational and Public Outreach Effort at UCSB

Philip Lubin
JPL 1289807 09/21/06-09/30/08 \$ 17,000
Planck Educational and Public Outreach Effort at UCSB

Philip Lubin
JPL 1289807 09/21/06-09/30/08 \$ 18,000
Planck Educational and Public Outreach Effort at UCSB

Philip Lubin
JPL 1289807 09/21/06-11/30/08 \$ 18,000
Planck Educational and Public Outreach Effort at UCSB

Jet Propulsion Laboratory Subtotal \$ 70,500

National Aeronautics & Space Administration

David Cannell
NNX08AE53G 03/01/08-02/28/2010 \$ 65,000
Gradient Driven Fluctuations

National Science Foundation

Guenter Ahlers
DMR-0702111 05/01/07-04/30/09 \$ 155,000
Turbulent Convection in a Fluid Heater from Below

Dirk Bouwmeester
PHY-0504825 08/01/05-07/31/08 \$ 120,000
Quantum Superposition States of a Mirror

Dirk Bouwmeester
PHY-0804177 08/01/08-07/31/09 \$ 280,000
NIRT: Quantum States of OptoMechanical Structures

Steven Buratto, Michael Bowers, Horia Metiu
CHE-00749489 04/01/08-03/31/09 \$ 202,000
Model Nanocluster Catalysts: The Role of Size, Shape and Composition on the Catalytic Activity on Monometallic, Bimetallic and Metal Oxide Clusters on Oxide Surfaces

Andrew Cleland
DMR-0605818 07/01/06-06/30/09 \$ 115,000
Mechanical Quantum Resonators: Quantum Optics with Phonons

Deborah Fygenson, Dirk Bouwmeester
CCF-062257 09/01/06-08/31/08 \$ 100,000
DNA Patterned Pairs of Colloidal Quantum Dots: A Scalable Approach to Computing Without Wires

Bruce Lipshutz
CHE-0550232 02/01/06-01/31/09 \$ 148,000
Asymmetric Catalysis with Ligated Copper Hydride

Mark Sherwin
DMR-0703925 07/01/07-06/30/09 \$ 130,000
Terahertz Electro-Optics and Intersubband Micro-Plasmonics in Semiconductor Quantum Well Devices

National Science Foundation Subtotal \$1,151,000

Oak Ridge National Laboratory

Douglas Scalapino

4000068439 04/14/08-09/30/10 \$ 210,666
Explorations of Routes to Higher Superconducting Transition Temperatures

Sandia National Laboratories

S. James Allen

784231 03/06/08-09/30/08 \$ 40,000
Terahertz Resonant Plasmonic Detectors

The Marine Research Institute (Iceland)

Bjorn Birnir

SB080063 11/01/07-10/31/09 \$ 64,548
Simulations of Complex Schools of Fish

UC Discovery Grant

Norbert Reich

Bio05-10524 01/12/07-04/24/08 \$ 2,623
Rapid Detection of HPV in Clinical Samples

UC Los Angeles

Michael Bowers

SB070075 09/01/06-07/31/08 \$ 260,582
Pathogenic Protein Folding and Human Disease

William M. Keck Foundation

Mark Sherwin, S. James Allen, Elliott Brown, Song-I Han, Philip Lubin, Kevin Plaxco, Mark Rodwell
SB080017 07/01/07-06/30/10 \$ 1,750,000
“Filming” Proteins in Action Using UC Santa Barbara’s Free-Electron Lasers

Research Support Summary (2007-2008)

Federal

| | | |
|---|--------------------|---------------|
| Air Force | \$189,000 | 4.36% |
| Army | \$224,470 | 5.17% |
| Department of Energy | \$165,375 | 3.81% |
| Environmental Protection Agency | \$15,007 | 0.35% |
| Jet Propulsion Laboratory | \$70,500 | 1.62% |
| National Aeronautics and Space Administration | \$65,000 | 1.50% |
| National Science Foundation | \$1,250,000 | 28.81% |
| Oak Ridge National Laboratory | \$210,666 | 4.86% |
| Sandia National Laboratories | \$40,000 | 0.92% |
| Federal Totals | \$2,230,018 | 51.40% |

International

| | | |
|-------------------------------------|-----------------|--------------|
| Marine Research Institute (Iceland) | \$64,548 | 1.49% |
| International Totals | \$64,548 | 1.49% |

Private/Other

| | | |
|-----------------------------|--------------------|---------------|
| Florida State University | \$31,014 | 0.71% |
| William M. Keck Foundation | \$1,750,000 | 40.33% |
| Private/Other Totals | \$1,781,014 | 41.05% |

State

| | | |
|---------------------------------------|------------------|--------------|
| UC Discovery Grant | \$2,623 | 0.06% |
| University of California, Los Angeles | \$260,582 | 6.01% |
| State Totals | \$263,205 | 6.07% |

| | | |
|---------------|--------------------|----------------|
| TOTALS | \$4,338,785 | 100.00% |
|---------------|--------------------|----------------|

Charts and Graphs

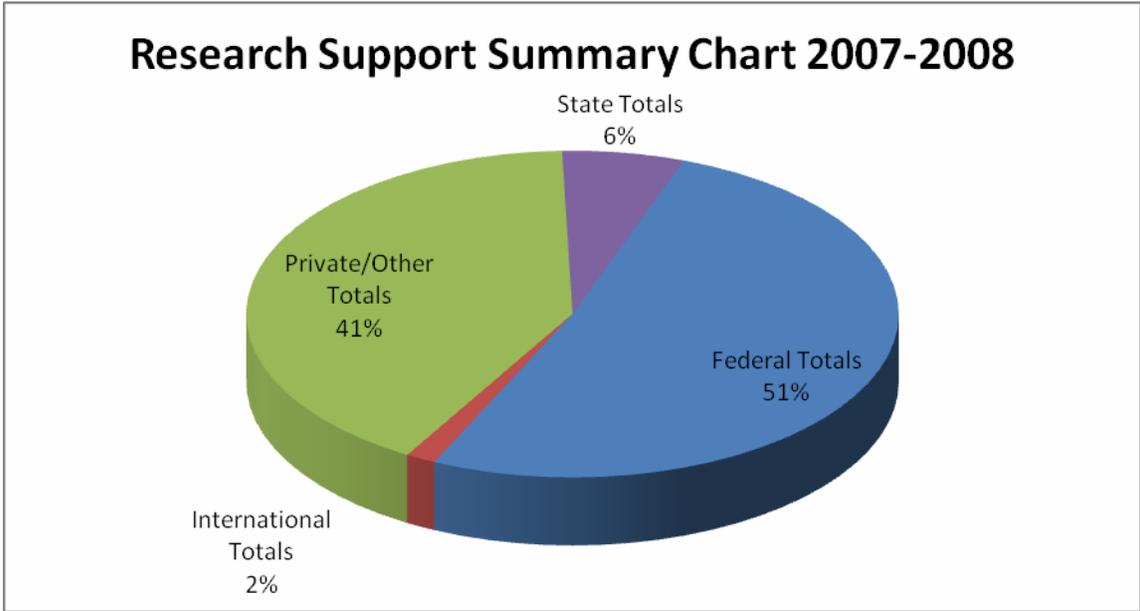


Chart 1: Research Support Summary Chart 2007-2008

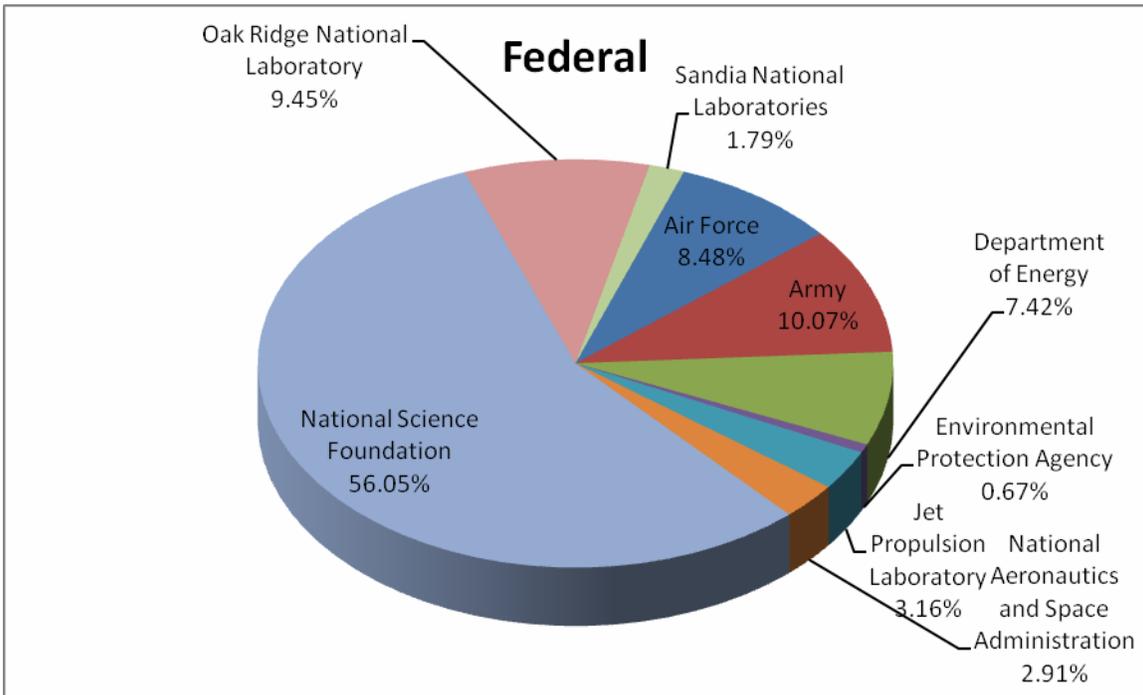


Chart 2: Federal Research Support Summary Chart

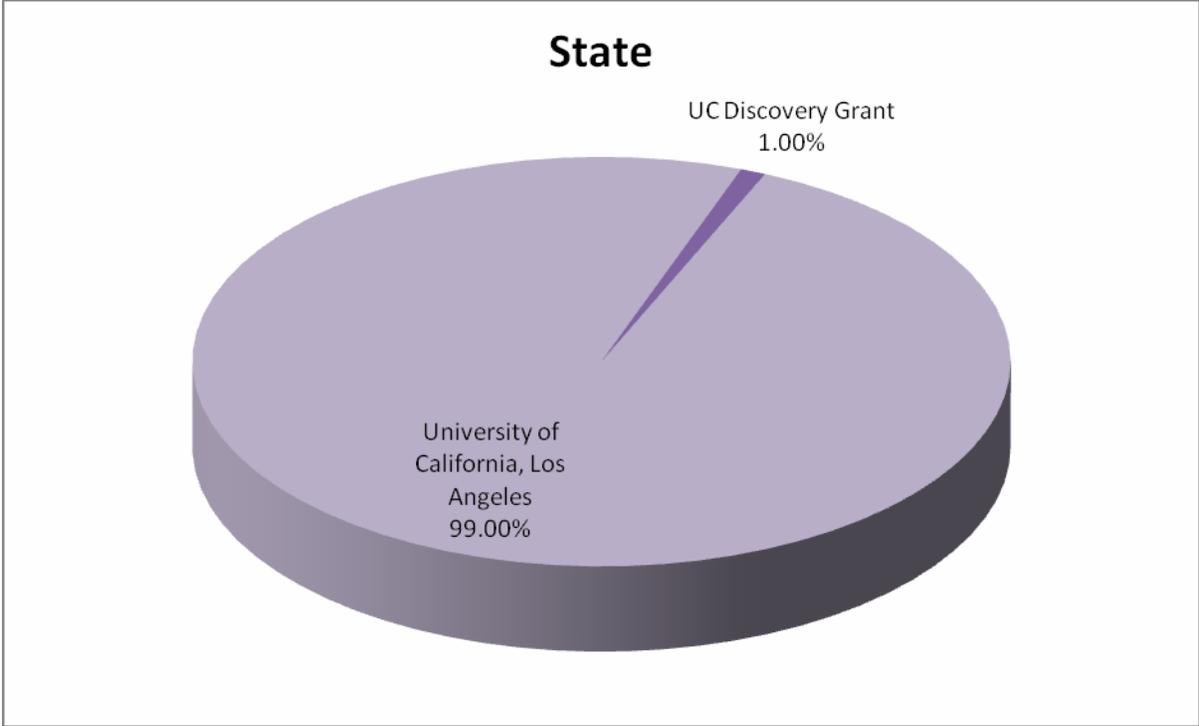


Chart 3: State Research Support Summary Chart

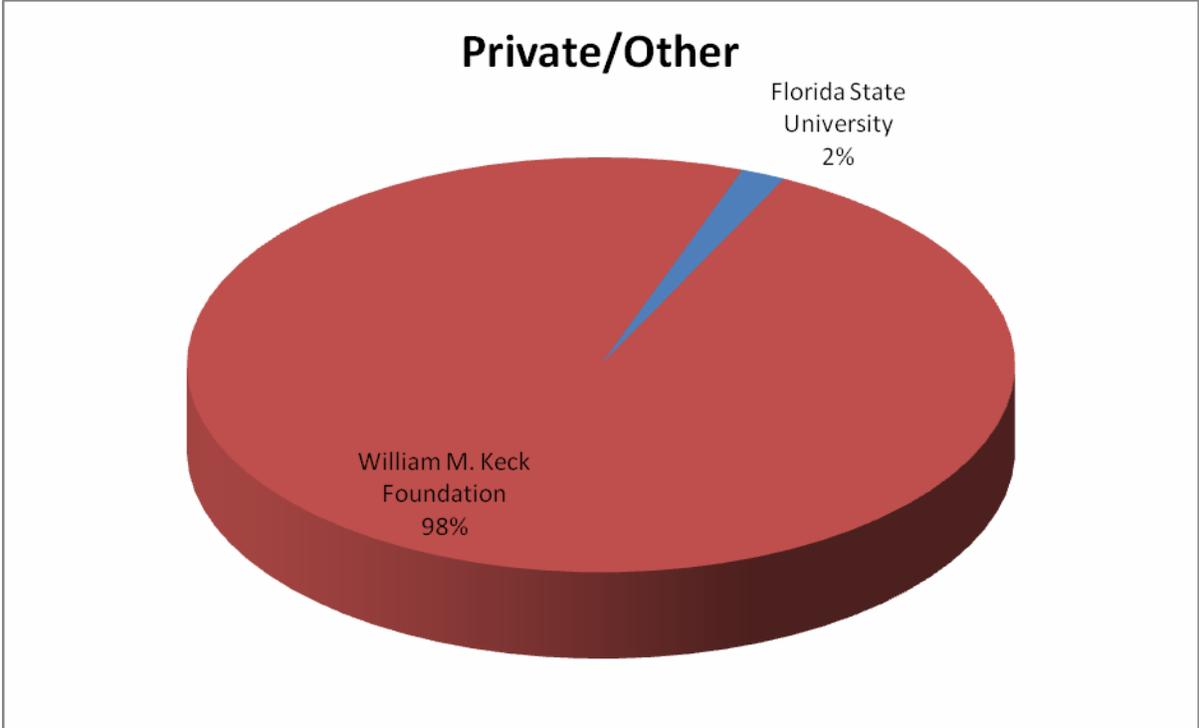


Chart 4: Private/Other Research Support Summary Chart

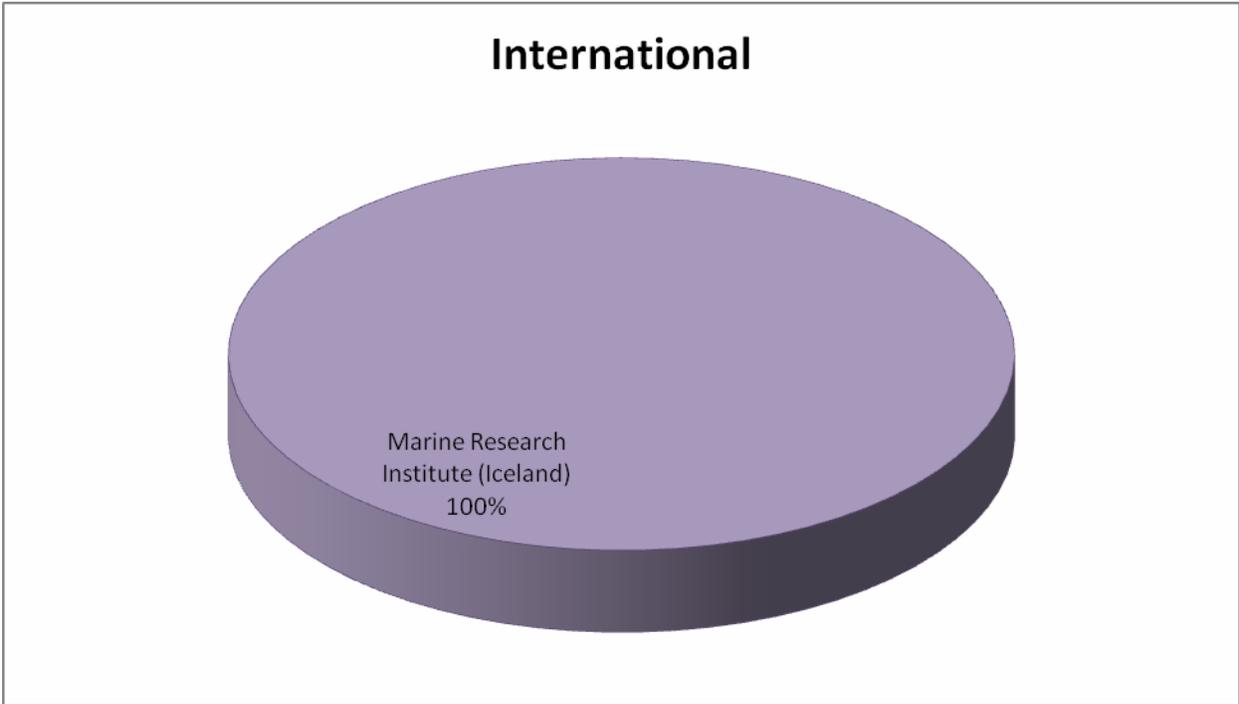


Chart 5: International Research Support Summary Chart

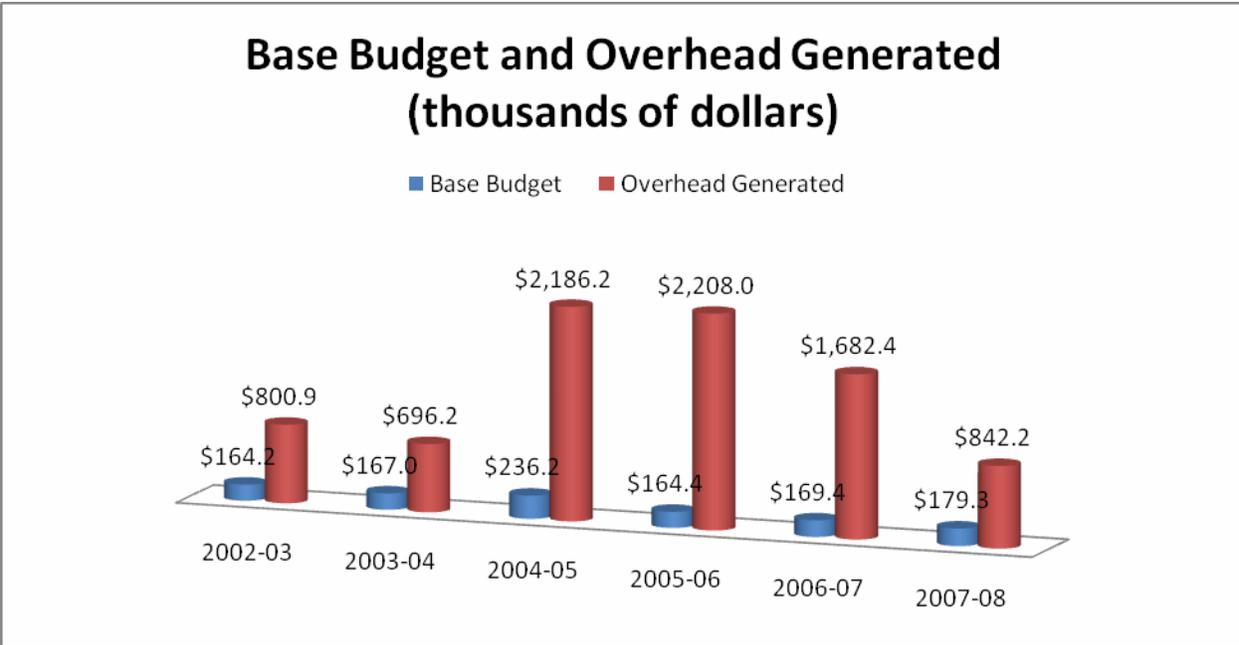


Chart 6: Base Budget and Overhead Generated

Number of Proposals Submitted and Funded

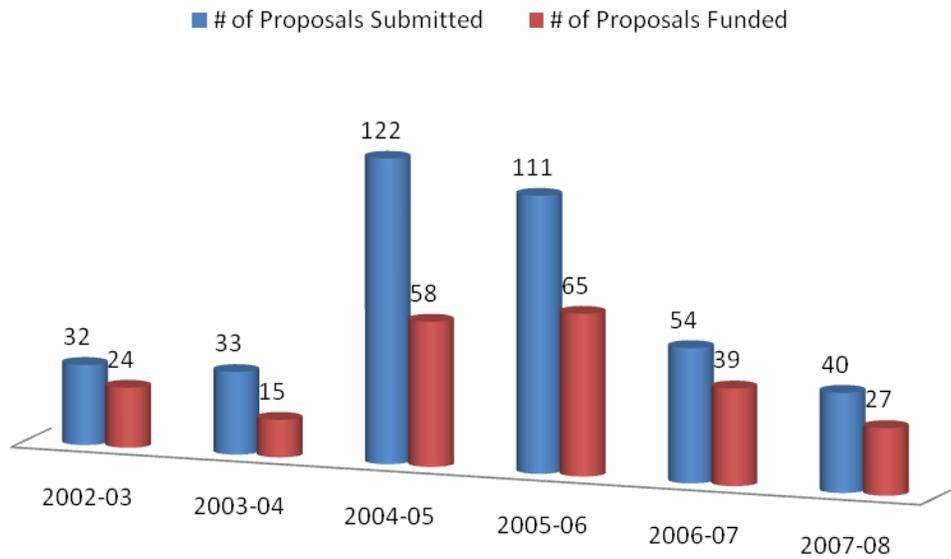


Chart 7: Number of Proposals Submitted and Funded

Value of Proposals Submitted and Funded (millions of dollars)

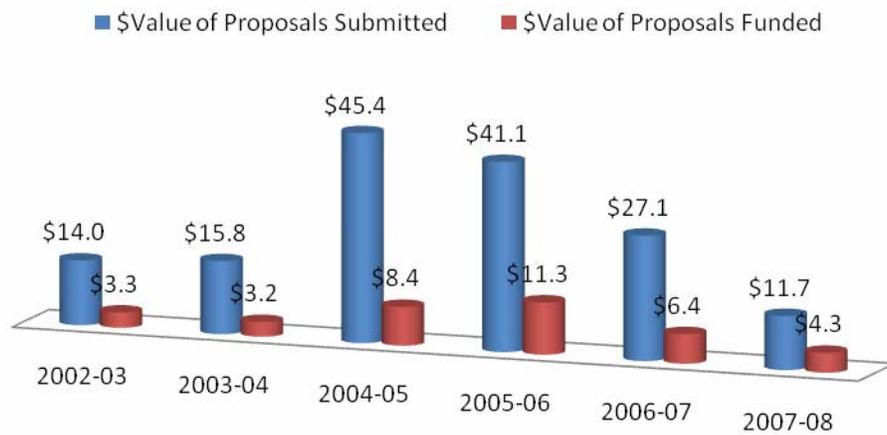


Chart 8: Value of Proposals Submitted and Funded

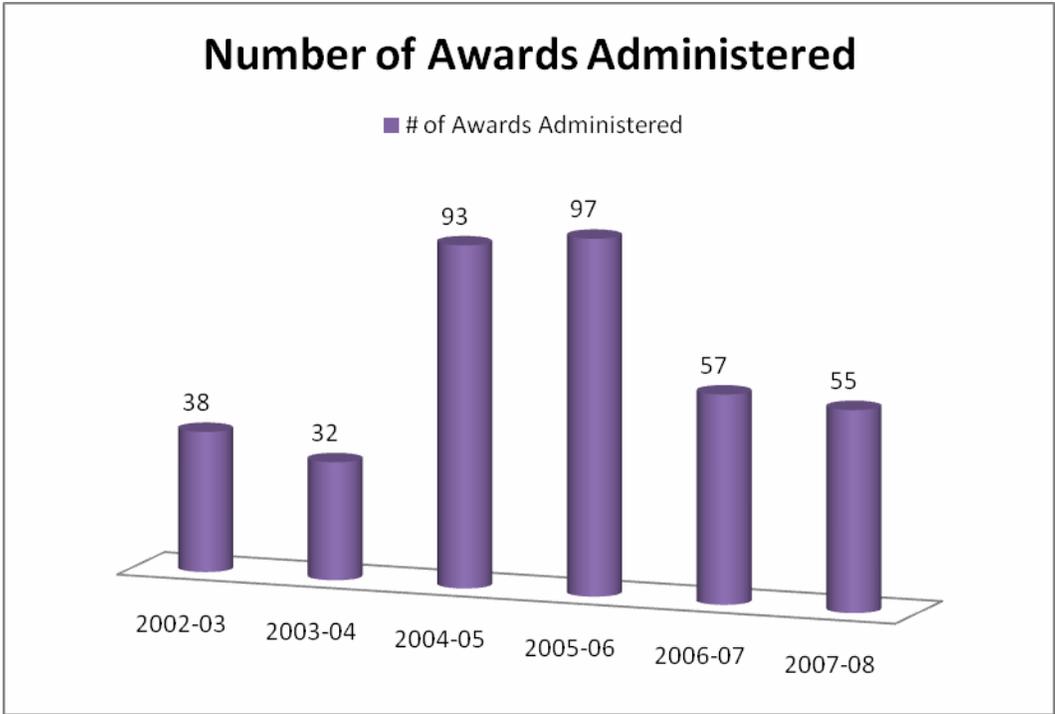


Chart 9: Number of Awards Administered



Chart 10: Value of Contracts and Grants Administered

Statistical Summary for iQCD

2007-2008

| | | |
|--|--|--------------|
| 1. Academic personnel engaged in research: | | |
| a. | Faculty | 40 |
| b. | Professional Researchers (including Visiting) | 8 |
| c. | Project Scientists | 1 |
| d. | Specialists | 6 |
| e. | Postdoctoral Scholars | 18 |
| f. | Postgraduate Researchers | 2 |
| | TOTAL | 75 |
| 2. Graduate Students: | | |
| a. | Employed on contracts and grants | 63 |
| b. | Employed on other sources of funds | 0 |
| c. | Participating through assistantships | 0 |
| d. | Participating through traineeships | 0 |
| e. | Other (specify) | 0 |
| | TOTAL | 63 |
| 3. Undergraduate Students: | | |
| a. | Employed on contracts and grants | 26 |
| b. | Employed on other funds | 2 |
| c. | Number of volunteers, & unpaid interns | 0 |
| | TOTAL | 28 |
| 4. Participation from outside UCSB: (optional) | | |
| 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 | 5 |
| b. | Administrative/Clerical | 5 |
| 6. Seminars, symposia, workshops sponsored | | 5 |
| 7. Proposals submitted | | 40 |
| 8. Number of different awarding agencies dealt with* | | 35 |
| 9. Number of extramural awards administered | | 55 |
| 10. Dollar value of extramural awards administered during year** | | \$20,037,413 |
| 11. Number of Principal Investigators*** | | 47 |
| 12. Dollar value of other project awards **** | | \$482,336 |
| 13. Number of other projects administered | | 7 |
| 14. Total base budget for the year (as of June 30, 2007) | | \$179,314 |
| 15. Dollar value of intramural support | | \$1,032,669 |
| 16. Total assigned square footage in ORU | | 10,582 |
| 17. Dollar value of awards for year (08 Total) | | \$4,338,785 |

* 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 |
| David Awschalom | Professor | Physics |
| Bjorn Birnir | Professor | Mathematics |
| Daniel Blumenthal | Professor | Electrical and Computer Engineering |
| Jeffrey Bode | Assistant Professor | Chemistry and Biochemistry |
| Dirk Bouwmeester | Professor | Physics |
| Michael Bowers | Professor | Chemistry and Biochemistry |
| Elliot Brown | Professor | Electrical and Computer Engineering |
| Thomas C. Bruice | Research Professor | Chemistry and Biochemistry |
| 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 |
| Patrick Daugherty | Associate Professor | Chemical Engineering |
| Michael Doherty | Professor | Chemical Engineering |
| Peter Ford | Professor/Vice Chair | Chemistry and Biochemistry |
| Deborah Fygenson | Associate Professor | Physics |
| Song-I Han | Assistant Professor | Chemistry and Biochemistry |
| Robert Jacobs | Professor | Pharmacology, Ecology, Evolution & Marine Biology |
| Luc Jaegar | Associate Professor | Chemistry and Biochemistry |
| John Lew | Associate Professor | Molecular, Cellular & Developmental Biology |
| Bruce Lipshutz | Professor | Chemistry and Biochemistry |
| Dan Little | Professor | Chemistry and Biochemistry |
| David Low | Professor | Molecular, Cellular & Developmental Biology |
| Philip Lubin | Professor | Physics |
| Eric McFarland | Professor | Chemical Engineering |
| Horia Metiu | Professor | Chemistry and Biochemistry |
| Martin Moskovits | Dean of Sciences | College of Letters and Science |
| John Perona | Associate Professor | Chemistry and Biochemistry |
| Pierre Petroff | Professor | Materials |
| Thomas Pettus | Associate Professor | Chemistry and Biochemistry |
| Kevin Plaxco | Professor | Chemistry and Biochemistry |
| Craig Pryor | Chief Scientist | Terahertz Device Corporation |
| Jerry Ramian | Research Specialist | iQCD |
| Norbert Reich | Professor | Chemistry and Biochemistry |

| | | |
|-------------------|----------------------|-------------------------------------|
| Mark Rodwell | Professor | Electrical and Computer Engineering |
| Douglas Scalapino | Research Professor | Chemistry and Biochemistry |
| Susannah Scott | Professor | Chemical Engineering |
| Mark Sherwin | Professor | Physics |
| Galen Stucky | Professor | Chemistry and Biochemistry |
| Petra van Koppen | Lecturer | Chemistry and Biochemistry |
| Jelena Vuckovic | Assistant Professor | Stanford University |
| Yoko Yamakoshi | Associate Researcher | Chemistry and Biochemistry |

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

