Chemical and Biomolecular Engineering research projects 2007-08

CPATH CB: Computing Across Curricula

Lisa Bullard, George Rouskas, Tom Miller, Jeff Joines, Amy Craig, Dianne Raubenheimer, Larry Silverburg, Eric Weibe, and Carol Miller
NSF
$258,749
2007-2010

The project has two overarching goals: (1) create a computational thinking thread in the engineering curriculum that spans from the freshman to senior years and bridges the divide between freshman year computing and computing in upper-level classes, and (2) enable students to take computing competency to the next level, where they are able to perform high-level computing tasks within the context of a discipline.

Ligands from Combinatorial Peptide Libraries for Pathogen Detection and Removal

Ruben G. Carbonell
American Red Cross
$2,800,000
2000-2008

Ligands that bind to prion protein from hamster brain homogenate in human blood and

plasma have been identified. These are now being incorporated into nonwoven fabrics to make filters that can be used for the processing of blood products. Additional work is being done to develop ligands that bind to viruses as well as detection and diagnostic

devices.

NSF Science and Technology Center for Environmentally Responsible Solvents and Processes

Ruben G. Carbonell and Joseph M. DeSimone
National Science Foundation
$36 million
1999-2009

This Center has just been renewed for the second five years of operation. Its major focus is on the use of high-pressure carbon dioxide as a solvent in the areas of microelectronics, polymer synthesis and processing, and nanoparticle production and assembly. The use of carbon dioxide would result in a reduction of millions of pounds per year in the use of aqueous and organic solvents in these critical industries. In addition, carbon dioxide offers some unique processing advantages due its low viscosity, high diffusivity and low surface energy. New facilities have been constructed to pursue the incorporation of carbon dioxide-based processes in microelectronics, including a 193 nm stepper in the Engineering Graduate Research Center. Additional information on specific research programs can be found at www.nsfstc.unc.edu.

Design of nanocarrier materials to be used in conjunction with viral vectors.

DeSimone, Joseph M. and Juliano, Rudolph
Pharmacology - The Pharmacodynamics of Genes and Oligonucleotides
NIH
$225,704 (DeSimone's)
5/1/05 to 3/31/10

The overall thrust of this program is to develop and evaluate technologies and strategies that will promote the effective utilization of antisense oligonucleotides, siRNA, and genes as therapeutic agents. The approach will draw upon exciting new developments in nucleic acids chemistry and biology, recent progress in targeted drug delivery, and emerging capabilities in nanotechnology. These themes will be brought together in a synergistic manner to create novel and effective delivery systems for oligonucleotides and genes.

NSF Science & Technology Center for Environmentally Responsible Solvents and Processes

DeSimone, Joseph M.
NSF
11/01/1999 to 10/31/2009
Total award $33,358,518; DeSimone (co-PI) $7,090,487; UNC $11,636,870

More than 30 billion pounds of organic and halogenated solvents are used worldwide each year as process aids, cleaning agents, and dispersants. Considerably more water is used and contaminated in related processes. Technological breakthroughs in the last decade now indicate that liquid and supercritical carbon dioxide could be the most commonly used solvents of the twenty-first century as the manufacturing and service industries attempt to avoid the production, use, and subsequent release into our environment of contaminated water, volatile organic solvents, chlorofluorocarbons and other noxious pollutants.

Develop methodology and successfully demonstrate polymerization of fluoromonomers in carbon dioxide: Polymerization of Fluoromonomers in Supercritical Fluids

DeSimone, Joseph M.
DuPont
$150,000 per year; Total award $2,485,217.40
12/17/1992- open

Dense carbon dioxide has been shown to be an excellent reaction medium for the synthesis of fluoropolymers. Indeed, significant advantages are found in the synthesis of tetrafluoroethylene (TFE) based polymers due to the increased safety in handling of the TFE as a mixture with CO2, as well as the environmental advantages over fluorocarbon solvents. Recent studies have shown that non-aqueous grade PFA and FEP can be synthesized readily in dense carbon dioxide.

Novel Perfluoropolyether Fouling Release Coatings: Investigations of Structure Property Relationships Relevant to Fouling Resistance and Release

DeSimone, Joseph M.
Office of Naval Research
$300,000
11/01/06 to 11/30/08

Current antifouling coatings are responsible for alarming increases in the levels of organotin and other toxic compounds in the vicinity of dry-docks, harbors and shipping lanes. As such, the work proposed herein seeks to establish use of perfluoropolyether (PFPE) release coatings as safe, nontoxic, environmentally benign alternatives to antifouling technologies. As a unique class of fluoropolymers, PFPE polymers and copolymers have been established as high performance materials, which combine low surface energies (12-15mN/m), low moduli, as well as excellent thermal and chemical stabilities with the practical ease of solution or solventless processibility.

Center for Cancer Nanotechnology Excellence

DeSimone, Joseph M. and Juliano, Rudolph
NIH - Lineberger Cancer Center
$2,407,965 3 yrs. Projects 1 & 2 (DeSimone)
9/1/05 to 8/31/2010

The major thrust of this proposal is to design and fabricate several types of novel nanodevices and to evaluate them in the context of powerful and informative biological models, with the emphasis on mouse tumor models. We believe that this will eventually result in rapid progress in translational research leading to novel diagnostic and therapeutic approaches to cancer. While several nanotechnologies are represented, the overarching research theme of our CCNE will be the design of smart nanoparticles. This focus is based on the emergence of a radical new approach to nanoparticle fabrication that was developed at the UNC Chemistry Department.

Proton Exchange Membranes for Next Generation Fuel Cells

DeSimone, Joseph M.
Department of Energy
$450,000
9/15/05 to 9/14/08

Pioneering approaches to the fabrication of two new classes of high performance polymer electrolyte membranes (PEMs) that exploit heretofore unprecedented levels of morphologic control will be developed and integrated into prototype fuel cells designed for next generation power sources. We will develop and tailor the properties of PEMs using the following methods: 1) Curable liquid precursors to very high acid containing PEMS; and 2) Exploitation of a new modular PEM design employing self-assembled block copolymers. The most successful candidates will be integrated to generate a revolutionary material that will be tested for performance as a prototype fuel cell.

Integrated Nanofluidic Electronic Sensor Technologies for Army Applications

DeSimone, Joseph M.
US Army Research Office
$3,006,000.00
8/15/2005 to 9/28/2008

This project is a new approach to develop integrated sensor systems for defense department and Army applications. The project will merge five pioneered concepts: (1) novel polymers for new generations of nano-moldable soft lithography MEMS nanofluidic components; (2) new proton exchange membranes and catalysts for fuel cells integrated into microfluidic devices; (3) artificial ligand-gated ion channel devices for identification and quantification of species at the single molecule level; (4) carbon-nanotube based nanoelectrochemical sensors and tailored microelectrodes; and (5) simulation and modeling tools for design of nanoscale devices for specialized sensor applications in the areas of Chemical and Biological Agent detection.

Research Agreement Between UNC and Liquidia in the Area of PFPE, Lithography, Mi

DeSimone, Joseph M.
Liquidia Technologies, Inc.
$817,819
09/01/2005 to 09/01/2008

Research agreement between UNC and Liquidia Technologies to perform research in the following areas: Characterization of PFPE-based elastomers; Imprint Lithography using PFPE-based patterned molds: Microfluidics; micro- and Nano-particles; and membrane studies.

Novel Imaging Probes – Design and of novel Fabrication Imaging Probes Utilizing PRINT

DeSimone, Joseph M. and Sartor, R. Balfour
NIH
$146,000
8/1/2006 to 7/31/2008

Utilization of the PRINT technology in this study will allow for a more detailed understanding of the overlapping roles of shape, size, mechanical and chemical functionality in the bio-distribution of carriers in vivo and will yield expertise needed for the preparation and use of target specific contrast agents for noninvasive early detection of inflammation and disease. Fabrication of novel nanoparticle loaded with contrast agents and functionalized with antibodies which recognize unique cellular components will be used for the noninvasive measurement of inflammation using magnetic resonance imaging in an in vivo mouse model.

Targeted PRINT nanoparticles for treatment of Type 1 diabetes.

DeSimone, Joseph M. and Frelinger, J.
JDFR
$73,000
9/1/2007 to 8/31/08

Type 1 diabetes (T1D) is a tissue specific autoimmune disease characterized by the T mediated destruction of the insulin producing b cells of the islets of Langerhans. Treatment of diabetes has focused on the use of insulin replacement. However, this treatment can be difficult to regulate and has many shortcomings. While the surgical techniques for transplanting pancreatic islets is now at hand, problems remain.

JamBots: Reconfigurable Chemical Robots

DeSimone, Joseph M. and Jaeger, H.
US Army/DARPA
$500,000
1/25/08-7/24/09

The team will work collectively to provide the foundation and the design of the key ingredients required for creating a "JamBot" capable of locomoting, morphing, and assembling a payload.

Nanoparticle Foundry

DeSimone, Joseph M. and Juliano, Rudolph
NIH - NC University Cancer Research Fund
$1,300,000
10/15/07 to 10/14/08

PRINT Particle Foundry activities consist of the design of master templates, fabrication and distribution of the nanoparticles to researchers. The PRINT technology allows us to be able to produce isolated nano-carriers and is the first and only general, singular method capable of forming particles that are monodisperse in size and concomitant uniform shape, which can be molded into any shape for which a master can be generated, from essentially any matrix material and can be functionalized with targeting ligands. The PRINT nanoparticles have a myriad of applications in diagnostics, early detection and treatment of any number of disease states.

Nanostructured Materials for Renewable Alternative Energy

Gregory Parsons, Orlin Velev, Michael Dickey, Veena Misra, Christopher Gorman
US Department of Energy
$ 625,916 ($ 77,273 Velev part, $ 100,000 Dickey part), Period covered:
07/25/2008 to 07/24/2009

The objective of this program is to achieve improvements in solar absorptivity and energy transduction in organic photovoltaic devices and to obtaining a detailed understanding of the fundamental relations between nanoscale structure and chemical composition for improving PV and other renewable energy systems. For example, new nanoscale patterning, self-assembly, and atomic-scale thin film coating techniques are being developed that can produce new high surface area inorganic and organic/inorganic hybrid materials systems useful for PV and other energy transduction platforms.

Lithium Alloy-Carbon Composite Nanofibers for Energy Storage by Electrospinning and Carbonization

Peter Fedkiw, Saad Khan, and Xiang-Wu Zhang
National Science Foundation
$380,000
9/1/06 to 8/30/09

Electrospinning and carbonization technologies are applied to integrate dissimilar materials (lithium alloy and carbon) into a novel type of composite nanofiber for use in lithium-ion batteries. The resultant nanofiber materials combine the advantageous properties of lithium alloy (high-storage capacity) and carbon (long-cycle life) in that the carbon matrix accommodates the volume change of the encapsulated lithium alloy nanoparticles during lithium insertion/extraction. The composite nanofibers are electrospun into nonwoven fabrics for use as lithium-ion anodes and thereby eliminate the present use of non-active materials resulting in improved energy and power densities.

Portable Power Based on Anion Exchange Polymer Membrane Fuel Cells

Peter Fedkiw
DuPont Company
$361,000
6/1/2009 to 5/31/11

Anion exchange membrane (AEM) fuel cells have the potential to utilize non-noble metal electrocatalysts for both the anode and cathode to replace the costly precious metals currently used in state-of-art cation exchange membrane fuel cells. In this project, we measure fundamental fuel-cell relevant properties of novel AEMs and assess their suitability for AEM fuel cells that use methanol as the fuel.

Evaluation of Hydrogen Production by Photosynthetic Bacteria, non-Photosynthetic Bacteria, Cyanobacteria, and Algae Immobilized Within a Latex Coating

M.C. Flickinger (Co-PI, NCSU), M. Siebert (Co-PI, NREL)
DOE National Renewable Energy Laboratory CRD-05-170 (extended)
$40,000
2/13/2006-2/12/2008 (on going)

This CRADA involves collaboration on development of nanostructured composite latex adhesive coatings for entrapment of the photosynthetic bacterium Rps. palustris, the green microalgae Chlamydomonas reinhardtii, non-photosynthetic bacteria and Cyanobacteria for their ability to survive the drying process and produce hydrogen following coating and rehydration.

Advanced Training in Growth, Physiology and Gene Transfer of Bacillus methanolicus

M.C. Flickinger (PI, NCSU)
Creavis Technologies, Evonik Degussa Corporation (Marl, Germany)
$84,000
9/15/2007-7/15/2008 (no cost extension to 3/31/2009)

This project involves training of one post doctoral associate for growth, genetic manipulation and high cell density fed-batch fermentation of the thermotolerant, methylotrophic Gram positive bacterium Bacillus methanolicus.

Production of Biofuels from Waste Gas Streams using Textiles Coated with Microbial Catalysts

M.C. Flickinger (Co-PI, NCSU), M. Chinn, A. Grunden, S. Peretti, K. Zering (Co-PIs, NCSU)
North Carolina Biotechnology Center
$269,055
7/1/2008 – 6/30/2010

This project involves development of nanostructured coatings of C. lungdahlii strains capable of converting CO and CO_2 to ethanol and acetate and acetoclastic methanogens for conversion of acetate to methane as useful fuels from gasified biomass. It involves microbial physiology studies to improve the ethanol selectivity, conversion of acetate to methane, investigation of nanostructured coatings to intensify and stabilize microbial reactivity, development of carbon flux models to predict the metabolic behavior of the microbial coatings as well as economic characterization of the efficiency of this conversion of biomass to useful fuels.

Encyclopedia of Industrial Biotechnology: Bioprocess, Bioseparation and Cell Technology

M.C. Flickinger, Editor-in-Chief (PI, NCSU)
John Wiley & Sons
$15,000
2005-2008 (no cost extension to 12/31/1009)

This is the equivalent of the Kirk-Othmer Encyclopedia of Chemical Technology, but for the industrial biotechnology industry. It will be published in print and also as an electronic encyclopedia in late 2009. >350 authors worldwide from industry and academia contribute to this work.

Bio-nanotechnology Undergraduate Laboratory in Engineering Education

Kirill Efimenko (PI, NCSU), Jan Genzer, Orlin Velev, Michael Flickinger (coPIs, NCSU)
North Carolina Biotechnology Center
$79,900
Feb 6, 2009 – Feb 5, 2010

The purpose of this program is to establish a new cross-disciplinary nanobioscience laboratory course. This laboratory course, which will serve annually ÿ-150 junior- and senior-year NCSU undergraduate students, will have the following primary goals: i) Introduce undergraduate students to hands-on experiences with current tools and practices in nanoscience and bio-nanotechnology; ii) teach undergraduate students how to apply fundamental principles of bio-nanotechnology for manufacturing commercially important products, and iii) engage students from different disciplines in working together in collaborative and cooperative learning activities, while developing problem-solving and applying technical communication skills research and product development.

Development of CO_2-Based Deposition Techniques for Production of Tunable Coatings on the Surfaces of Elastomers

Jan Genzer
NSF STC Center at NCSU
$28,500
11/1/2008 to 10/31/2009

The major theme of this project is to develop techniques for attaching semifluorinated organic modifiers from supercritical CO_2 to poly(dimethylsiloxane) network (PDMS-N) surfaces and study their physico-chemical properties.

Random-blocky copolymers: Monomer sequencing through templated chemical coloring

Jan Genzer
NSF-DMR
$520,106
2/1/2004 to 9/30/2009

The central theme of the proposed research plan is to demonstrate the ability of random-blocky copolymers (RBCs), heteropolymers with statistically controlled monomer sequence distributions, to undergo self-assembly in the bulk and perform recognition of chemical patterns on surfaces. We plan to establish that controlling the statistical nature of the sequencing is sufficient in endowing the RBC with unique assembling and recognition characteristics; these may allow the RBC to perform functions similar to those of more complex biomolecules

Development of combinatorial polymeric substrates for fast and efficient screening of protein adsorption

Jan Genzer
NSF-CTS
$270,038
7/1/2004 to 8/15/2009

Engineers at NC State University and scientists at BD Technologies aim to develop a novel technology platform for investigating protein adsorption on material surfaces. We plan to exploit a combinatorial screening methodology that improves upon existing analytical tools by enabling faster, more reliable, and more efficient evaluation of protein adsorption. This new approach will provide an effective analytical method and will facilitate manufacturing of devices with controllably modified biointerfacial properties.

Nanomolecular Interactions of Novel Biological and Synthetic Polyelectrolyte Brushes

Alan Grodzinsky (PI, MIT), Christine Ortiz (co-PI, MIT), Jan Genzer (co-PI), Igal G. Szleifer (co-PI, Northwestern U.)
NSF-NIRT
$1,700,000 ($417,499 for J. Genzer)
7/1/2004 to 8/31/2009

The overall goal of this research proposal is to use powerful new nanoscale experimental and theoretical tools and methodologies to develop a foundation for the fundamental physics of novel technologically important polyelectrolyte brush and brush-like systems. An interdisciplinary research team includes 4 PI's representing 5 academic departments at 3 universities who have expertise in a broad array of fields including; tissue structure and biomechanics, biochemical analysis, electrical engineering, mechanical engineering, bioengineering, electrostatic double layer continuum theory, nanomechanics, surface science, polymer mechanics, materials science and engineering, surface science, polymer physics, directed self-assembly, chemical engineering, statistical mechanics of complex fluids, computer simulations.

Combinatorial polymeric substrates: Analytical platform for adsorption, separation and functional assay of biological molecules

Jan Genzer (PI, NCSU), Evangelos Manias (co-PI, PSU), Richard Vaia (co-PI, AFRL), Andrea Liebmann-Vinson (co-PI, BDT)
ONR
$1,193,000 ($460,899 for J. Genzer)
1/1/2005-4/15/2010

The objective of our work is to provide steps towards a design and fabrication of multipurpose sensing/separation device; the general applicability of such a device for detecting various bioprobes stems from the general functionality of our design that is based on the combination of a physical and chemical separation. Development of these methods will lead to the creation of nanostructured devices that preserve functionality of the biological species and thus serve as a platform for robust extraction and separation of various antigens. The specific goals of the work encompass understanding the underlying phenomena that give functionality

to such a device.

How does substrate geometry affect the surface-initiated "living" polymerization?

Jan Genzer
ACS PRF
$131,625
9/1/2007-8/31/2009

We use Monte Carlo simulations to study the effect of the substrate geometry (flat vs. concave vs. convex) on "grafting from" polymerization via "living"/controlled radical mechanism. The specific goals include probing the initiator surface grafting density, monomer concentration, life-time of the "living" radicals, and termination probability on polymer molecular weight and polydispersity index. The simulation results reveal important and experimentally hard-to-determine information about the structure of the brush close to the substrate and will reveal how "grafting from" differs (at least in its initial stages) from the conventional bulk polymerization.

Design of multivariant polymeric substrates for studies of biomolecular adsorption and cell signaling

Jan Genzer (PI, NCSU), Jason Haugh (co-PI, NCSU)
ARO
$510,846
2/1/2007-1/31/2010

The principal theme of the proposed work is to study how adsorption, signaling, and proliferation of fibroblast cells depend on physico-chemical properties of substrates, including, surface chemistry and substrate compliance. Substrates will be designed and fabricated that comprise gradual and continuous variation of chemical characteristics of surfaces and their elastic modulus. By integrating two individual gradient building blocks, one involving chemical nature and one comprising gradual variation of the substrate elastic modulus, we will produce complex gradient motifs, where each individual position on the substrate reflects a unique combination of the two independently varying properties.

PIRE: POLYMER Education and Research Partnership between US and Korea

Chang Ryu (PI, RPI), Jan Genzer (coPI, NCSU) & 3 other coPIs
NSF-PIRE
$2,500,000
Aug 15, 2007 – Aug 14, 2012

A coherent multi-university team with the faculty members from several US universities (RPI, UMass at Amherst, Univ. of Texas at Austin, Princeton, and NCSU) is working together to develop a global research and education endeavor in polymer synthesis, characterization, and theory by forming the PIRE partnership with (1) Korean language/culture training specialist, in the US, and (2) faculty members at several Korean universities (POSTECH, Seoul Nat. Univ., Sogang Univ., and Yonsei Univ). The proposed US-Korea partnership will promote collaborative research activities on heteropolymers with adjustable monomer sequences (HAMS).

Construction of Kerr Effect Apparatus for Polymer Characterization

Jan Genzer (PI, NCSU), Bruce Novak & Al Tonelli (coPIs, NCSU)
DURIP-ARO
$81,525
Jul 1, 2008 – Jun 30, 2009

The purpose of this program is to build a unique instrument capable of measuring the so-called Kerr effect in heteropolymers. The new Kerr effect apparatus will be the first of its kind that will be solely dedicated to characterizing the properties of heteropolymers (i.e., macromolecules bearing more than one chemical unit). Kerr effect measurements will provide a unique means to characterize polymer conformations, comonomer sequences, polymer tacticity, and composition of various heteropolymer systems.

Long-Lived Antifouling Coatings by Mechanical Assembly of Grafted Molecules and Buckling Underlying Soft Foundations

Jan Genzer
ONR
$328,766
Oct 1, 2006 – Sep 30, 2009

The central theme of this proposal is: i) to prepare coatings with tunable characteristics by utilizing two variants of the "mechanically assembled monolayer" (MAMs) method, and ii) to demonstrate that these coatings possess good antifouling properties. The MAMs technology is based on combining mechanical deformation of silicone elastomer network sheets, modifying their surfaces with ultraviolet/ozone treatment, and chemically grafting organosilane moieties.

Bio-nanotechnology Undergraduate Laboratory in Engineering Education

Kirill Efimenko (PI, NCSU), Jan Genzer, Orlin Velev, Michael Flickinger (coPIs, NCSU)
North Carolina Biotechnology Center
$79,900
Feb 6, 2009 – Feb 5, 2010

The purpose of this program is to establish a new cross-disciplinary nanobioscience laboratory course. This laboratory course, which will serve annually ≈100-150 junior- and senior-year NCSU undergraduate students, will have the following primary goals: i) Introduce undergraduate students to hands-on experiences with current tools and practices in nanoscience and bio-nanotechnology; ii) teach undergraduate students how to apply fundamental principles of bio-nanotechnology for manufacturing commercially important products, and iii) engage students from different disciplines in working together in collaborative and cooperative learning activities, while developing problem-solving and applying technical communication skills research and product development.

In-Plane Nanostructural Organization of Copolymer Molecules Along Polymer/Polymer Interfaces

Richard Spontak (PI, NCSU), Jan Genzer (coPI, NCSU)
NSF
$105,127
Aug 1, 2008 – Jul 31, 2009

The in-plane (lateral) interfacial structure of polymer/polymer interfaces in thin-film polymer laminates is critical to the development of advanced coatings, in which case the

molecular-scale conditions responsible for promoting film stabilization must be fully established and understood. The primary objective of this project is to elucidate the type and extent of lateral structuring of diblock copolymers at interfaces between two immiscible homopolymers and how lateral interfacial structuring develops.

The Use of Environmentally Benign Sequestrants for the Removal of Scaling Mineral Deposits

Christine S. Grant
National Science Foundation: GOALI
$270,000
2004-2008

This research investigates the role of mass transfer and surface reactions on the dissolution of mineral films (i.e., barite, calcium phosphate, calcium carbonate) using sequestrant solutions in neutral and alkaline environments. Fundamental interfacial mechanisms describing the interaction of the sequestrant ligand with the minerals is key to understanding reactions at the surface and in the bulk solution. Continued research on the use of polyaspartic acid as an environmentally benign dissolution agent has led to industrial interactions with BP Corporation; providing an important link to both the chemical and pharmaceutical processing industries.

ADVANCE LEADERSHIP AWARD: Peer Mentoring Summits for Women Engineering Faculty of Color (African-American, Hispanic, Native American)

Christine S. Grant
National Science Foundation
$299,995
5/06 – 4/09

Women of Color (WOC) are significantly underrepresented on U.S. engineering faculties; a 2002 study, of chemical engineering at the top 50 departments, indicates WOC are less than 0.75 % of the reported ChE faculties. This program leads improvement of recruitment/retention by addressing unique issues at the intersection of race and gender, with a series of "summits/mini-summits". The goals are to identify best practices for successful recruitment, retention and promotion and creating peer mentoring networks for WOC in engineering academia. In 2007, over 60 women attended the summit –2009 summits for Senior Women Leadership (NCSU) and all faculty ranks (Caltech).

NSF Sustainability, Energy and Engineering Research Experience for Undergraduates (REU) Site

S. W. Peretti and Pamela Martin; Martin Hubbe and C.S. Grant
National Science Foundation
$ 450,000
1/06 – 1/10

This REU award for a 4 year site on environmentally sustainable products and processes, and energy supports 11 undergraduate students per year in a 10-week research and professional development program at NCSU. The objectives of this REU Site are threefold: (1) to develop future knowledge leaders in sustainability and green engineering; (2) to enhance the likelihood of successful graduate education in students from predominately undergraduate institutions and groups underrepresented in engineering; and (3) to develop in the participants disciplined thinking related to science, as well as the ethical and economic motivations for implementation of science for sustainable manufacturing practices.

Extend and Assess Research Ethics Education

Chi Anyansi-Archibong (NCA&T), Brenda Alston-Mills, Christine Grant, Gary Comstock, A. Ayanna Boyd-Williams (NCA&T): Co-PIs
National Science Foundation
$ 299,999
9/07 – 8/10

First national effort to disseminate a standardized, interdisciplinary, inter-institutional, collaborative online curricular intervention in research ethics; the project extends and assesses research ethics education in 3 ways: a) Extend the "OpenSeminar in Research Ethics" doctoral course from two of the doctoral-degree granting universities in the UNC system to all seven doctoral campuses; b) Assess the effectiveness of the OpenSeminar in achieving its pedagogical goals across the system; c) Establish a mechanism/template for extending the OpenSeminar to other state systems. It encourages high ethical standards preparing students for globally inter-connected world where cultural differences and expectations can raise daunting dilemmas.

BE-MUSES/Collaborative Research: Health Protective Textiles: Bridging the Disposable/ Reusable Divide

Christine Grant (MR Overcash – Former PI)
National Science Foundation
$345,263
9/04 – 8/09

As infectious diseases circle the globe, skyrocketing medical costs and waste streams require a comprehensive assessment of medical textiles (e.g., protective performance, costs, health risks and environmental impacts). The selection of reusable and disposable textiles is determined by many factors, such as costs, protective and comfort properties, government regulations, and social and psychological perceptions of both textiles. Specific research objectives are to: (1) determine the most effective, multi-functional (biocidal and water-repellent) materials for medical applications; (2) quantify how economic, environmental, and health risk reduction impacts healthcare textiles usage; (3) determine social/psychological factors affecting acceptance of new material by healthcare workers.

The Model Curriculum for Land Grant Universities in Research Ethics (LANGURE)

Gary Comstock, Brenda Alston-Mills and C.S. Grant
National Science Foundation
$ 249,393
2005-09

LANGURE's ultimate aim is to institutionalize the teaching of research ethics. It's the first interdisciplinary, inter-institutional initiative; creating a national network of eight land-grant universities (LGUs) and historically black colleges and universities (HBCUs) teaching research ethics to doctoral candidates in engineering and the physical, social and life sciences. Based at NCSU, faculty and graduate students will conjointly develop a one-credit course, "Introduction to Research Ethics". LANGURE will develop a suite of 15 interactive, online research-ethics modules including: statistics, nanotechnology, physics, chemical engineering,

computer science, intellectual property, and the role of women and underrepresented minority students in engineering and scientific research.

NSF: AGEP (Alliances for Graduate Education and the Professoriate) Collaborative Research Training: North Carolina Alliance to Create Opportunity Through Education (OPT-ED)

David Shafer and John Gilligan; Christine S. Grant (Senior Personnel)
National Science Foundation
$51,000 (Allocated to CSG project); (Total Grant: $657,216)
3/05– 2/10

OPT-ED's goal is to substantially enhance efforts in NC to increase the number of underrepresented minority (URM) students receiving PhD degrees and ultimately entering the professoriate in science, technology, engineering, and mathematics (STEM). The project includes all NSF-HRD supported URM initiative projects in NC: Louis Stokes Alliance Minority Participation Program, Historically Black Colleges and Universities, and Centers for Research Excellence in Science and Technology, and North Carolina Math Science Education Network. OPT-ED will have a broad impact across several educational levels, and the state of North Carolina. The PURPOSE Institute is responsible for URM faculty conducting professional development seminars to mentor undergraduate/graduate students.

Paradigm Shift Towards Positive Outcomes in Orthopedic Events for Ageing Diverse Populations

Christine S. Grant (lead)
The National Academies Keck Futures Initiative (NAE/ NAS/ NIM)
$50,000
5/08-6/10

The project investigates increasing successful orthopedic outcomes for culturally diverse patients through: (i) a health navigator to interface with patients and medical systems negotiating primary care/medical issues, (ii) intersection of future (K-12) doctors with an ageing population in faith based communities highlighting the importance of their potential presence in the profession (iii) improved understanding/application of the important role faith has in an ageing patient's rehabilitation, commitment and interaction with medical professionals. The multidisciplinary team of: orthopaedic clinicians, biomedical, public health researchers, spirituality/medicine/health and elderly orthopaedic wellness experts culminates in a national invited roundtable forming expert partnerships for a comprehensive program.

Molecular Modeling of Confined Nano-Phases and Nano-Porous Materials

Keith E. Gubbins
NSF, NRAC
$125,000/year
11/1/02 to 10/31/08

The work under this project is aimed at understanding the behavior of fluids in porous media, in particular the effects of such confinement on phase transitions, chemical equilibria and transport properties. Current projects being pursued are studies of shifts in the freezing transition in porous carbons, improved molecular models of activated carbons, effect of confinement on diffusion rates in carbons, and the influence of pore size, material and state conditions on chemical reaction equilibria. These large simulations are carried out on supercomputers at several NSF national centers (San Diego, Illinois and University of Texas) under a large NRAC grant.

NIRT: Surfactant Self-Assembly on Nano-Structured Surfaces: Multi-Scale Computational Prediction and Design

Keith E. Gubbins (PI), Jerzy Bernholc (co-PI), Don Brenner (co-PI) and Sharon Glotzer (University of Michigan, co-PI)
$1,300.000
09/01/04 to 08/31/09

Multi-scale strategies are being developed to study soft matter systems, particularly the self-assembly of non-ionic surfactants on solid surfaces and in nanoporous materials. These strategies, based on quantum mechanics, atomistic molecular dynamics, and meso-scale dynamics are aimed at bridging these three scales of distance and time, and so bringing to bear a methodology for rigorously studying the kinetics, thermodynamics and structure of these nano-scale structures. The team involved in this project includes Keith E. Gubbins (PI), and co-PI's Donald Brenner (NCSU, Materials and Engineering Science), Jerzy Bernholc (NCSU, Physics) and Sharon C. Glotzer (University of Michigan).

US-Germany Cooperative Research: Surfactant Self-Aggregation on Solid Surfaces and in Pores

Keith E. Gubbins
NSF
$22,006
9/15/2003 to 8/31/2008

This is a cooperative research project between Professors G.H. Findenegg, M. Schoen and S. Klapp at the Technical University of Berlin, and Professor K.E. Gubbins at NCSU. The research is aimed at understanding and quantitatively predicting the wide variety of nano-structures formed when non-ionic and ionic surfactants self-assemble on solid surfaces and in pores. These structures are of potential applications as sensors, in photonics and in electronic devices, but their formation and behavior is poorly understood, and is often anomalous in the sense that they do not behave in a manner that is expected based on the behavior of simpler molecules. Experiments and meso-scale simulations are being carried out by the team in Berlin. Atomistic and electronic level simulation studies are being carried out in Raleigh. The grant provides support for travel between Raleigh and Berlin for faculty, postdoctoral workers and graduate students.

GOALI: Molecular Modeling of Confined Nano-Phases and Novel Nano-Porous Materials

Keith E. Gubbins
NSF
$300,000
10/01/2006 to 09/30/2009

This is a GOALI project involving university-industry collaboration between North Carolina State University and Quantachrome Instruments, a leading manufacturer of instruments for characterizing nano-structured materials. The aim of the project is to develop and apply atomistic simulation methods to obtain realistic atomic models of several new classes of synthetic nano-porous materials, and to use

these to investigate confined phases within these materials, as well as to optimize the materials themselves. The materials under study include templated silicas, mesoporous carbons and periodic mesoporous organosilicas. Experimental studies of these materials are being performed at Quantachrome Instruments, while atomistic simulation studies are being pursued at NCSU.

Porous Carbons: A Complementary Experimental and Molecular Modeling Study

Keith E. Gubbins
ARO
$141,400
07/01/2007 to 09/30/2010

This is a synergistic research program that combines experimental tools and molecular modeling methods, with the goal of developing realistic models of nanoporous carbons, and understanding the adsorption behavior of various adsorbates, in particular water. Our collaborators at the Army Research Laboratory will gather experimental data, including structure factors and adsorption data. Molecular simulation studies, including Hybrid Reverse Monte Carlo and Grand Canonical Monte Carlo calculations, will be carried out at NCSU. The results of these studies will be used to develop optimal materials for adsorption, particularly in the presence of humidity.

US Poland Workshop on Interfacial Phenomena and Advanced Materials

Keith Gubbins
NSF
$49,683
10/01/2007 to 09/30/2009

This grant provided support for U.S. participants to attend a 3 day Workshop on "Interfacial Phenomena and Advance Materials," held in Gdansk, Poland on June 4-6, 2008. The purpose of the Workshop was to encourage closer scientific contacts and long term research collaboration between researchers in this area between the U.S. and Poland. The Workshop involved 15 U.S. participants and 15 from Poland, with a balance between junior, mid-career and senior researchers, and between experiment and theory, with similar or complementary interests on the two sides. In addition, young researchers in these areas from Poland attended the meeting, presented poster papers, and interacted with the more senior participants throughout the meeting.

Collaborative Research: Removal of Toxic Gases by Intercalation and Reactice Adsorption

Keith Gubbins
NSF
$122,075.00
04/01/2008 to 03/31/2011

In this project work we are investigating and designing novel reactive adsorbents for the removal of toxic gases from air streams. We use a combined experimental and theoretical approach to explore toxic gas removal using reactive adsorption, by designing graphite oxide materials with functional surface groups that are optimal for removal of these gases. The experimental work is being carried out at CUNY City College by Professor T.J. Bandosz and coworkers, and the theoretical work is done at North Carolina State University. We seek to determine the fundamental mechanism, at the atomic and electronic levels, of reactive adsorption/intercalation of small molecule toxic gases on these materials.

Multi-Scale Modeling of Reaction with Diffusion

Keith Gubbins
ACS
$100,000.00
07/01/2008 to 08/31/2010

In this project multi-scale modeling methods will be employed to understand the role of chemical kinetics, diffusion and adsorption for reactions to produce hydrogen from low molecular weight hydrocarbons. Ab initio calculations based on density functional theory will be used to determine potential energy surfaces for these reactions on carbon substrates with and without transition metal catalysts. The results of these calculations will be used to carry out atomistic molecular dynamics calculations using rare event MD to determine the rates of reaction with diffusion. The extent to which diffusion is limiting will be determined for various ordered and disordered materials.

Molecular Modeling of Adsorption and Diffusion in Ordered and Disordered Nano-Porous Materials

Keith E. Gubbins
Department of Energy
$150,000/year
02/01/05 to 01/31/09

Molecular simulation methods are being used to study adsorption and diffusion in both ordered and disordered nano-porous materials of interest to the energy industry. Three areas are emphasized. The first is the development of realistic molecular models for templated mesoporous materials (TMM's) and activated carbons, using mimetic simulation and reconstruction techniques. The second area is the investigation of the behavior of water and water/alkane mixtures in activated carbons, with varying types and concentrations of surface oxygenated sites present. Third, the selective adsorption of sulfur compounds from air and gas streams will be studied.

Adsorption of Small Molecule Gases on Graphite Oxide Based Materials: Exploring the Mechanism of Combined Intercalation and Reactive Adsorption

National Science Foundation
Teresa J. Bandosz (City College New York) and Keith E. Gubbins (co-PI)
$145,257
04/01/2008 – 03/31/2011

In this project the goal is to develop functionalized graphite oxides and graphite oxide-metal oxide framework (MOF) nano-composites as reactive adsorbents for the removal of toxic industrial gases, including ammonia, chlorine and sulfur oxides, from air streams. The materials combine the strong adsorption properties of carbons with the chemisorption behavior of MOF's. Experimental studies are being carried out at CCNY, and theretical studies at the ab initio and semi-classical levels are carried out at NCSU.

Computer Simulation Studies of Protein Aggregation

National Institutes of Health
Carol Hall
$813,524
12/1/04 -11/30/08

The aberrant assembly of proteins into amyloid fibrils is a cause of many different human disorders including Alzheimer's and Parkinson's . An understanding of the

molecular-level mechanisms that result in the aggregation of proteins into amyloid is essential for the discovery of potential therapeutic strategies and diagnostics. The project has three specific aims: (1) to learn the basic physical principles governing protein fibrillization, (2) to shed light on the molecular mechanisms responsible for the aggregation of polyglutamine, and (3) to investigate the aggregation of specific amyloidogenic peptides by extending a previously-developed model, PRIME, to all 20 amino acids .

Bioengineering Research Partnership on Aggregation of Therapeutic Proteins: A Subcontract

University of Colorado: A Subcontract on a National Institutes of Health Grant
Carol Hall
$665,503 (Hall portion)
9/15/2006 – 8/31/2011

This proposal established a Bioengineering Research Partnership aimed at understanding how to control and/or inhibit the aggregation of therapeutic proteins. The PI is Ted Randolph of the University of Colorado. Hall is conducting molecular–level computer simulations that complement and inform the experiments and mathematical modeling of the other partners. She contributes to the following aims: (1) to determine the dependence of protein aggregation rates on conformational and colloidal stability as a function of pH, ionic strength, and the concentration of excipients, and (2) to determine how chemical modification of peptides affects their conformational and colloidal stabilities, and aggregation kinetics.

Computational Discovery of Complex Nucleic-acid-based Architectures for Nanoengineering

National Science Foundation
$1,500,000
9/01/2008- 8/31/2012
PI (C. Hall) Co-PIs (P Agris, S. Craig, T LaBean)

DNA based self-assembling nanomaterials offer great potential for bottom-up assembly of designed complex nanomaterials, with applications in a diverse range of disciplines. This multidisciplinary team is using a cyber-driven strategy to design highly-cooperative complex three-dimensional architectures in solution and at planar and nanoparticle surfaces using modified natural and non-natural nucleosides. The project has three specific aims: (1) to predict the structure and stability of selected two- and three-dimensional DNA-based nanoscale building blocks, (2) to predict the relative stability of DNA-based structures on planar surfaces and/or with metallic nanoparticles and (3) to predict new, hybrid extended three-dimensional architectures.

Novel Peptide Intervention Targets a Critical Host-Retrovirus Molecular Interaction

North Carolina Biotechnology Center
$63,588 (Hall portion)
12/01/2008- 11/20/2010
PI (P Agris) Co-PIs (A Dieters, C. Hall and F. J. Fuller)

The long-term goal of this project is to develop a novel antiviral therapeutic against any lentivirus infections, including HIV, that targets the unique properties of the host cell $tRNA^{Lys3}$ recruitment by viral protein for priming reverse transcription. Twenty small, 15- and 16- residue amino acid peptides have been identified that bind to the chemically rich portion of the anticodon domain of $tRNA^{Lys3}$. Molecular dynamics simulations (modeling) of the peptide/$tRNA^{Lys3}$ interaction is being conducted to improve the peptide affinity and specificity for tRNA, and to provide insight into the types of small molecules that would inhibit viral protein interactions with tRNA.

Molecular Crosstalk in Intracellular Signaling Networks

Jason Haugh
NIH-General Medical Sciences, R01-GM067739
$710,180
9/1/03 - 8/31/08

In this project, we aim to combine quantitative experimentation and mathematical modeling to analyze crosstalk interactions between the Ras-Erk and PI 3-kinase/Akt intracellular signaling pathways, which are centrally involved in cell proliferation and survival. Correlations between molecular-level perturbations of those pathways and the resulting cell responses will also be sought.

Signal Transduction in Models of Fibroblast Invasion

Jason Haugh
NIH-General Medical Sciences, R21-GM074711
$356,555
5/16/06 - 5/15/09

This exploratory proposal was submitted under PA-03-058, Exploratory/ Development (R21) Bioengineering Research Grants (EBRG). The goals of the project are to develop integrated mathematical models, informed by experiments, of intra- and inter-cellular communication and the resulting effects on fibroblast invasion, a critical process in wound healing.

Cell Migration Consortium - Modeling Initiative Outreach Collaboration

Jason Haugh
Univ. of Virginia (subcontract through the Cell Migration Consortium NIH glue grant)
$346,020
8/1/06 - 7/31/11

Our role in this large-scale, collaborative project is to study activation and regulation of Rho family GTPases, a critical process in establishing cell polarity during directed cell migration, using various computational modeling and simulation approaches. On the one hand, microscopic models of molecular assembly and enzymatic processes are being developed using Brownian dynamics and rule-based kinetic modeling methods, while on the other, macroscopic, cell-level descriptions of symmetry breaking and polarization of signal transduction are being developed and analyzed using standard, partial differential equation models.

Integrative Analysis of Cell Signaling Systems Across Multiple Levels of Biological Complexity

Jason Haugh
Camille & Henry Dreyfus Foundation, Camille Dreyfus Teacher-Scholar Award, TC-05-022
$75,000
5/15/05 - 5/14/10

This award provides discretionary funds to faculty at early stages in their careers. Criteria for selection included an independent body of scholarship and a commitment to

education. The PI is to develop a research and teaching program using wound healing as an example of multi-scale modeling and experimentation.

Design of Multivariant Polymeric Substrates for Studies of Biomolecular Adsorption and Cell Signaling

Jason Haugh (Co-PI) and Jan Genzer (PI, NCSU)
Army Research Office
$510,846
3/1/07 - 2/28/10

The principal theme of the proposed work is to study how adsorption, signaling, and proliferation of fibroblast cells depend on physico-chemical properties of substrates, including surface chemistry and substrate compliance. Substrates will be designed and fabricated that comprise gradual and continuous variation of chemical characteristics of surfaces and their elastic modulus. By integrating two individual gradient building blocks, one involving chemical nature and one comprising gradual variation of the substrate elastic modulus, we will produce complex gradient motifs, where each individual position on the substrate reflects a unique combination of the two independently varying properties.

Signaling Vector Analysis of Cell Migration

Jason Haugh
NSF-CBET, # 0828936
$300,000
9/1/08 - 8/31/11

This project offers i) a new conceptual framework for thinking about control of fibroblast migration at the level of intracellular signal transduction and ii) novel tools for quantitatively analyzing it. If successful, the proposed work would more generally unify distinct cell migration stimuli and behaviors in terms of common signaling dynamics.

Inexpensive, Nonfluorinated Anions for Lithium Salts and Ionic Liquids for Lithium Battery Electrolytes

Wesley Henderson, Peter Fedkiw, Michel Armand
Department of Energy
$703,146 ($476,033 for W. Henderson)
4/24/09-3/31/12

Plug-in hybrid electric vehicles (PHEVs) require cheaper Li-ion batteries with extended (5+ year) lifetimes and improved safety. We will develop and characterize new classes of inexpensive, nonfluorinated anions for Li battery electrolytes which will achieve many of the goals needed for new advanced Li batteries suitable for PHEVs and stationary energy storage applications.

Biomass Processing Using Ionic Liquids for Jet Fuel Production

Wesley Henderson
Air Force Office of Scientific Research
$331,629
3/1/08-2/28/11

This project will address a critical need of the U.S. Air Force, namely the production of jet fuel from the renewable domestic resource lignocellulosic biomass. The research will explore the use of ionic liquids as solvents for the pretreatment of biomass materials. This project will prepare a diverse range of ionic liquids to identify the role of cations and anions in biomaterial dissolution, examine biomaterial solubility and separation/recovery and examine the activity of cellulase enzymes in ionic liquids for the conversion of cellulose to D-glucose.

ResZwit (Resonance Zwitterion) Additives for Ionic Liquid Electrolytes

Wesley Henderson
Army Research Office
$150,000
8/15/07-8/14/10

Ionic liquids are of strong interest as replacements for molecular solvents in Li battery and electrochemical capacitor applications due to improved safety and high/low temperature performance relative to currently used electrolytes. Unfortunately, the ionic conductivity of ionic liquid-based electrolytes tends to be lower than current electrolytes which limits the power which may be obtained. New additives are being explored which may improve the ionic conductivity without compromising the other properties obtained through the use of ionic liquids.

Cryostrat and Nitrogen Generator for Powder XRD Characterization of Electrolyte Phase Behavior

Wesley Henderson
Army Research Office - DURIP
$89,450
4/20/09-4/19/10

An Oxford Cryosystems Cobra non-liquid nitrogen cryostream and Nitroflow Lab nitrogen generator will be added to an existing Bruker D5000 powder diffractometer with a Highstar area detector. The cryostat will enable temperature control of the powder diffractometer over a wide temperature range thus permitting a detailed exploration of Li battery and capacitor electrolyte phase behavior.

Thermal Instrumentation for Characterization of Biomass Processing Using Ionic Liquids for Jet Fuel Production

Wesley Henderson
Air Force Office of Scientific Research - DURIP
$150,000
4/20/08-4/19/09

Thermal instrumentation (DSC, TGA and rheometer) was acquired enabling the detailed characterization of the phase behavior, thermal stability and viscosity of ionic liquids and their mixtures with various biomass constituents (and model compounds) greatly aiding in the development of methods to convert lignocellulosic biomass into hydrocarbon fuels.

High Resolution Raman Spectrometer for Characterization of ResZwit (Resonance Zwitterion) Additives for Ionic Liquid Electrolytes

Wesley Henderson
Army Research Office - DURIP
$150,000
4/20/08-4/19/09

A high resolution Raman spectrometer with a heating/cooling stage was acquired to enable the characterization of ion and additive molecular conformations and ionic association interactions in the electrolytes with and without the additives. The additives are intended to decrease the viscosity and increase the conductivity of ionic liquid and ionic liq-

uid-lithium salt electrolytes for electrochemical capacitors and Li batteries. The spectroscopic information is highly complementary to viscosity, ionic conductivity, ion diffusion and volatility measurements.

Biotransformations Near and Above 100°C: Hyperthermophilic microorganisms and enzymes for bioenergy conversion

Robert M. Kelly and Michael W.W. Adams (Univ. of Georgia)
National Science Foundation
$440,000 (RMK)
9/1/2006 to 8/31/2009

This project continues a long-standing collaborative effort between the University of Georgia and North Carolina State University that focuses on hyperthermophilic enzymes and biocatalysis at extremely high temperatures. A functional genomics approach, based on cDNA microarray analysis, is being used to identify novel biocatalysts of significance for bioenergy conversion.

Graduate Training in Biotechnology

Robert M. Kelly, PI + 30 other NCSU faculty
National Institutes of Health
$1,356,805
7/1/2005 to 6/30/2010

Graduate training in biotechnology is provided through a multidisciplinary program involving NCSU faculty in four colleges. Students are supported for a two-year period during which they take lab-based biotechnology courses, courses in research ethics, professional development and biotechnology design. An industrial rotation and service project are also completed during this period.

Graduate Training in Molecular Biotechnology

Duane Larrick and Robert M. Kelly
Department of Education
$127,881
8/15/2007 to 8/14/2010

Graduate training in biotechnology is provided through a multidisciplinary program. Students are supported for a three-year period during which they take lab-based biotechnology courses, courses in research ethics, professional development and biotechnology design.

Functional approaches for annotating secretome-bound small ORFs in microbial genomes

Robert M. Kelly
National Science Foundation
$318,777
10/01/2007 to 9/30/2010

The goal of this project is to use "omics" tools for identifying and characterizing the functional products of small open reading frames in genomes of hyperthermophilic microorganisms.

Biohydrogenesis in the Thermotogales

Robert M. Kelly, Paul H. Blum (University of Nebraska-Lincoln), Kenneth Noll (UConn)
Department of Energy
$1,600,000 ($525,000 to RMK)
9/15/2008 to 9/14/2011

This project focuses on the mechanisms of peptide and sugar fermentation to molecular hydrogen by members of the bacterial order Thermotogales.

Novel hydrolytic enzymes from thermophilic anaerobes (BESC)

Robert M. Kelly, Michael W.W. Adams and Janet Westpheling (University of Georgia)
$875,000 to RMK
11/01/2007 to 9/30/2012
ORNL/Department of Energy Bioenergy Science Center

The goal here is to identify and characterize novel thermophilic microorganisms and enzymes that are effective in biomass deconstruction.

Uranium mobilization by extremely thermoacidophilic archaea

Robert M. Kelly, Paul H. Blum (University of Nebraska-Lincoln)
Defense Threat Reduction Agency
$1,050,000 ($525,000 to RMK)
4/9/2009 to 4/08/2012

This project focuses on microorganisms that are capable of mobilizing uranium from pyritic ores, using functional genomics and molecular genetics tools.

Development of a sterilization time-temperature integrator (TTI) based on enzymes from hyperthermophilic microorganisms

Robert M. Kelly and Josip Simunovic (NC State Food Science)
Center for Advanced Packaging and Processing Studies (CAPPS)
$66,000
6/1/2009 to 5/31/2010

The objectives of this project include the development of enzyme-based sensors to track sterilization trajectories in aseptic processing.

Metabolic engineering studies of extreme thermoacidophily

Robert M. Kelly, Paul H. Blum (University of Nebraska-Lincoln)
National Institutes of Health
$900,000 ($450,000 to RMK)
8/1/2009 to 7/31/2012

This project addresses the molecular and physiological basis for microbial life at high temperatures and low pH.

High Throughput Melt Electrospinning of Nanofibers using Supercritical Carbon Dioxide

Nonwoven Cooperative Reseach Center (NCRC)
Saad A. Khan, Juan Hinestroza and Behnam Pourdeyhimi
$150,000 (direct cost)
1/09 to 12/11

The proposed research focuses on establishing a novel methodology to electrospin nanofibers from polymer melts directly, without the use of solvents, and exploiting the plasticizing effect of supercritical carbon dioxide.

Electrospun Nanofibers of Enzymatically-modified Polysaccharide for Drug Delivery and Wound Healing

Nonwoven Cooperative Reseach Center (NCRC)
Saad Khan and Benham Pourdeyhimi
$120,000 (direct cost)
7/06 to 7/09

The proposal aims at fabricating nanofibrous matrix of natural polysaccharides, particularly guar galactomannan, for applications as vehicles for oral drug delivery and wound healing. The distinct feature of our approach lies in combining the inherent advantages of electrospun nanofibers with that of guar. Nanofibers facilitates faster/controlled drug release owing to their high surface to volume ratio. Guar is ideally suited for this purpose because of its natural abundance, low cost, bio -compatibility and -degradability, FDA approval, and ability to be enzymatically modified.

Lithium Alloy-Carbon Composite Nanofibers for Energy Storage by Electrospinning and Carbonization

National Science Foundation
Peter S. Fedkiw, Saad A. Khan and Xiangwu Zhang
$380,000
9/06 to 9/09

The objective of this research is to use electrospinning and carbonization technologies to integrate dissimilar materials (lithium alloy and carbon) into a novel type of composite nanofibers for energy storage. Carbon materials, commonly used in present lithium-ion batteries, suffer from the low theoretical capacities although they generally have long cycle lives. Lithium alloys have high capacities but their cycle lives are low due to the large-volume changes during lithium insertion/extraction. The nanofibrullar nonwoven materials produced through our approach will combine the advantageous properties of lithium alloy and carbon, for potential use as anodes in a lithium-ion battery.

Fundamentals of Fiber Formation

Nonwoven Cooperative Reseach Center (NCRC)
Russel Gorga, and Saad A. Khan
$120,000 (direct cost)
1/07 to 7/10

In melt-spinning polymer fibers, orientation and crystallinity can be developed by both the spinning and drawing processes. As such there is a critical need to obtain a fundamental understanding of the physics of spinning and drawing processes. This project focuses on developing 1) a predictive model for orientation developed during melt spinning of polymers and 2) a system of analytical techniques that can be employed to compare experimental data obtained to validate the model.

Electrospinning of Nanoparticle templated Nanofibers

NSF S&T Center
Saad Khan
$200,000
8/06 to 10/09

We examine a new approach to synthesize and incorporate metal nanoparticles into electrospun polymer nanofibers wherein the electrospinning polymer acts as both a reducing agent for the metal salt precursor, as well as a protecting and templating agent for the ensuing nanoparticles. The effects of process variables and material properties on the characteristics of the electrospun fibers are being deciphered.

Conversion of Biodiesel Derived Glycerol to Glycidol, Glycerol Carbonate and C3 Oxygenates by Catalytic and Biocatalytic Pathways

S. W. Peretti, H. H. Lamb, A. O. Hobbs, K. S. Creamer
USDA
$1,606,265
1/06– 12/09

Glycerol is a byproduct of biodiesel production that currently is in over-supply worldwide. Efficient conversion of glycerol to valuable chemical intermediates would improve biodiesel economics and provide bio-based alternatives for petroleum feedstocks. In this project, we are investigating the catalytic synthesis of glycidol, glycerol carbonate and 1,3-propanediol from glycerol. Glycidol (2,3-epoxy-propanol) is an intermediate in the production of polymers, adhesives, and surfactants, and enantiopure glycidol can be used in the synthesis of pharmaceutical compounds. Glycerol carbonate and 1,3-propanediol are relatively new “green” chemicals that have a variety of potential applications.

Mathematical Modeling of the Simultaneous Hydrolysis and Fermentation of Corn Starch to Ethanol

H. Henry Lamb
Novozymes
$50,000
2/07-2/09

U.S. bioethanol production is undergoing rapid expansion driven by high petroleum prices and government incentives for biomass-derived alternative fuels. In this project, we are investigating the simultaneous enzymatic hydrolysis of corn starch and fermentation of the resulting glucose to ethanol by yeast (Saccharomyces cerevisiae). The goal is to optimize the batch process to achieve maximum ethanol productivity while making efficient use of added alpha-amylase and glucoamylase enzymes. This project involves detailed mathematical modeling using laboratory kinetics data on enzymatic liquefaction and saccharification and yeast growth kinetics on glucose to predict ethanol productivity and yield.

High-Value Transportation Biofuels from North Carolina Feedstocks

William Roberts, H. Henry Lamb, Larry Stikeleather
Biofuels Center of North Carolina
$200,000
7/1/08-6/30/09

The overarching goal of this project is to further develop toward commercialization an innovative thermocatalytic process for converting bio-based fats and oils (triglycerides) into biofuels. Researchers at North Carolina State University (NCSU) have invented a patent-pending multi-step process trademarked Centia™ to convert fats/oils from a variety of biological sources, including plant oils and animal fats, into hydrocarbon fuels with physical and combustion characteristics virtually identical to petroleum-derived fuels. A variety of NC feedstocks will be converted to renewable diesel, jet fuel, and gasoline, including chicken fat, hog fat (lard) and canola oil.

Cross-college collaboration: Engineering with Languages, Education, and Design

D.F. Ollis
NSF
8/1/04 to 7/31/08
$300,000. (NSF DTS Award)

Use "take-apart" device lab to enrich courses in other colleges.

Integrated Molecular Layer Deposition and Atomic Layer Deposition of Organic and Inorganic Thin Films

Gregory Parsons PI
NSF – CBET
$300,000
6/01/06 to 5/31/09

This project focuses on physical and chemical requirements to routinely deposit and combine organic and inorganic thin film materials with bulk and interface quality required to significantly advance the fields of molecule-based electronic and optoelectronic devices. The work will expand the emerging field of molecular vapor deposition including study of covalently bound organic monolayer and multilayer polymeric films, as well as combining molecular vapor deposition with atomic layer deposition to achieve integrated organic/inorganic heterostructures.

Selective Bio-Molecule Filtration Media Formulated Using Vapor Phase Deposition Technology

Gregory Parsons PI
NSF – Subcontract from Alditri Technologies
$50,000
1/01/08 to 6/30/09

This project is working to understand and apply vapor-phase deposition technology to the production of well-defined coatings on nonwoven fibers, and to test feasibility of modified fibers as an advanced platform for chemically specific removal of toxins from fluid streams. The work addresses fundamental understanding of mechanisms associated with chemical modification of non-reactive hydrophobic surfaces to expand understanding of vapor-phase surface chemical modification and lead to new applications for modified fiber structures.

Nanostructured Materials for Advanced Alternative Energy

Gregory Parsons PI, 4 other co–PI's
DOE National Energy Technology Laboratory
Energy Efficiency and Renewable Energy Industrial Technology Program
$1,230,000
7/25/08 to 7/24/09

The objective of this program is to achieve improvements in solar absorptivity and energy transduction in organic photovoltaic devices and to obtaining a detailed understanding of the fundamental relations between nanoscale structure and chemical composition for improving PV and other renewable energy systems. For example, new nanoscale patterning, self-assembly, and atomic-scale thin film coating techniques are being developed that can produce new high surface area inorganic and organic/inorganic hybrid materials systems useful for PV and other energy transduction platforms.

Surface Engineering of Nonwoven Materials using Atomic Layer Deposition and Self-Assembled Nanolayers

Gregory Parsons
Nonwoven Cooperative Research Center
~$90,000
Jan 1, 2008 to Dec 31, 2010

This project focuses on applications of atomic layer deposition technology for coating and modifying fibers and fiber based systems. The goal is to understand how surface modification influences the function and performance of modified fiber-based materials, including bulk mechanical properties. We also work to identify unique challenges related to reactant transport and reaction kinetics in thin film formation in complex fibrous systems. Specific coated samples are delivered to industrial collaborators for evaluation and analysis.

Atomic Layer Deposition on 3D Fibrous Structures

Gregory Parsons
NSF Science and Technology Center for Environmentally Responsible Solvents and Processes
~$70K/year
Nov 1, 2006 to Oct 31, 2009

This project addresses challenges in low temperature atomic layer deposition for conformal coatings on natural and polymer-based fiber materials with very large surface areas. Of particular interest is the relationship between macroscopic material properties on large planar surfaces and microscopic material properties on nanostructured 3D fiber networks. We recently found that when a 3D system is coated with inorganic polar materials, insight into microscopic material conformality and homogeneity can be obtained using angular dependent infrared transmission spectroscopy. Analysis of coatings on non-planar structures is of interest for surface modification for bio–scaffolds as well as protective fiber systems.

Hybrid Organic/Inorganic Thin Films

Gregory Parsons
NSF Science and Technology Center for Environmentally Responsible Solvents and Processes
~$70K/year
Nov 1, 2006 to Oct 31, 2009

Novel vapor deposition approaches are being investigated for deposition of hybrid organic/inorganic thin films. For example, For this study, zinc oxide based hybrid materials are being formed in our group using Molecular Layer Deposition and Atomic Layer Deposition technologies. This method utilizes alternating dosing of diethyl zinc and ethylene glycol, in combination with diethyl zinc and H_2O, to investigate feasibility of forming these novel conformal materials. Expected applications include low–temperature surface modification and advanced electro–optic materials and devices.

Silver Deposition and Coating by ALD

Gregory Parsons
Silver Research Consortium
$30K
May 1, 2009 to April 30, 2010

Thin film deposition of silver materials on fibrous substrates, and coating of encapsulation layer onto silver surfaces are being investigated by atomic layer deposition. Silver thin

film materials are of interest for advanced conductive fiber applications, as well as sensing and biocidal coatings. Silver encapsulation is important for corrosion resistance and stability.

Conversion of Biodiesel Derived Glycerol to Glycidol, Glycerol Carbonate and C3 Oxygenates by Catalytic and Biocatalytic Pathways

S. W. Peretti, H. H. Lamb, A. O. Hobbs, K. S. Creamer
USDA
$1,606,265
1/06– 12/09

Glycerol is a byproduct of biodiesel synthesis from the triglycerides comprising oils and fats. Efficient conversion of glycerol to valuable chemical intermediates would improve biodiesel economics and provide bio-based alternatives for petroleum feedstocks. In this project, we will investigate the catalytic synthesis of glycidol, glycerol carbonate and glycerol carbonate esters from glycerol. Racemic glycidol (2,3-epoxy-propanol) is an intermediate in the production of polymers, adhesives, and surfactants, and enantiopure glycidol can be used in the synthesis of pharmaceutical compounds. Glycerol carbonate and glycerol carbonate esters are relatively new "green" chemicals that have a variety of potential applications.

Pilot Plant to Enhance Sustainable Conversion of Biomass to Ethanol Fuels in North Carolina

S. W. Peretti, A. O. Hobbs
Golden LEAF Foundation
$1,500,000
4/2007– 4/2010

We will construct and operate a pilot-scale biorefinery at the Lake Wheeler Road University Field Laboratory to convert waste biomass resources into fuel ethanol and other value-added chemicals. This facility will be used to develop new technology, integrate operations, optimize system performance and demonstrate the feasibility of producing ethanol from different biomass resources. Capable of processing hundreds of pounds per day, it will be used for teaching and developing the work force that can support this emerging business, as well as by in state business interests to evaluate and optimize process performance and improve economics.

Production of Biofuels from Waste Gas Streams using Textiles Coated with Microbial Catalysts

Mari S. Chinn,. Michael C. Flickinger, Amy M. Grunden, Steven W. Peretti, Kelly D. Zering
North Carolina Biotechnology Center
$243,977
7/2008-6/2010

The project will improve the efficiency of converting synthesis gas into marketable fuels and increase the feasibility of thermochemical fuel production in a biorefinery by: 1) Improving ethanol selectivity of effective autotrophic bacteria; 2) investigating nanostructured polymer coating formulations coated onto textiles to concentrate microbial activity and preserve viability at ambient temperatures; 3) Developing carbon flux models describing the metabolic behavior of these select biocatalysts for use in guiding future genetic and metabolic manipulations; and 4) Creating models that describe the economic characteristics and efficiency of the proposed biocatalytic coated textiles conversion processes.

Biomass Production and Chemical Composition of Ultra Low Alkaloid Tobacco 22ND-X1

R Long, D Danehower, R Parker, R Qu, R Lewis, S Peretti
22nd Century Limited
$317,550
4/2005 – 12/2009

Plants are capable of producing an intriguing array of primary and secondary metabolic products. Many of these products could add value to biofuels produced from the residual lignocellulose, starch, and sugars that plants contain. Green plants have been shown to be capable of producing much higher grade protein products. These products would be competitive with casein or even egg white ovalbumin, and could improve co-production economics dramatically. The research program is focused on development of field and process technologies that would recover these higher value protein co-products from green plant biomass.

Biodiesel Pilot Plant Outreach Upgrade@NCSU
S Peretti, A Hobbs
Biofuels Center of North Carolina
$198,385
04/2009 - 10/2010

A well instrumented 150 gallon pilot plant has been built at the Lake Wheeler University Field Laboratory. Upgrading this pilot plant for additional capability would allow NCSU students to explore methods of obtaining optimum methanol recovery, reduce water and energy consumption via improved wet and dry cleanup processes, develop novel techniques for processing waste oil resources and demonstrate essential analytical technologies to provide for good process quality control for biodiesel processing while reducing the atmospheric volatile organic air emissions and waste water stream discharges.

A Microfluidic System for Affinity Reagent Generation and Assay Development for High-Throughput Biomarker Validation

Balaji Rao (subcontract) and Kapil Pant, CFD Research Corporation (PI)
US Army MRMC
$8,858 (to Rao)
10/01/08 to 01/31/09

These funds were allocated to extend the first phase of a project with the overall objective of developing of a microfluidic platform for generating affinity reagents for biomarker candidates. The proposed effort involved the design and development of a microfluidic device to select proteins that bind their targets with high affinity, from combinatorial libraries.

A Microfluidic System for Affinity Reagent Generation and Assay Development for High-Throughput Biomarker Validation

Balaji Rao (subcontract) and Kapil Pant, CFD Research Corporation (PI)
US Army MRMC
$240,000 (to Rao)
02/01/09 to 01/31/11

This is the second phase of a project with the overall objective of developing of a microfluidic platform for generating affinity reagents for biomarker candidates. Such a platform will accelerate the process of biomarker validation and verification. The proposed effort involves the design and development of a microfluidic device to select high affinity

reagents from combinatorial libraries. Further, the microfluidic platform will be adapted to develop biomarker assays, using the high affinity probes generated.

A hyperthermophilic protein scaffold for engineering molecular recognition

Balaji Rao (PI)
Faculty Research and Professional Development (FRPD) award
$6,000
07/01/08 to 06/30/09

Antibodies are the most commonly used binding molecules in biomolecular measurement. However, antibodies have several disadvantages such as low thermodynamic stability, a large multi-domain structure stabilized by disulfide bonds and high cost of production. As an alternative to antibodies, we will use a protein from the hyperthermophilic archaeon Pyrococcus furiosus as a stable scaffold for engineering molecular recognition, i.e. a "template" for generating protein variants that bind with high affinity and specificity to target species.

Surface Biofunctionalized Polymer Nanofibers by Electrospinning

Richard J. Spontak
MeadWestvaco Inc.
$50,000
2007 to 2008

Nanofibers surface-modified with bioactive groups give rise to the production of bioactive materials for specialty textiles and biomedical applications. The objective of this research is to develop a process route wherein bioactive sequence-defined oligopeptide conjugates could be synthesized separately before being co-electrospun with other homopolymers into fibers. Surface enrichment of oligopeptides is achieved due to different polarizability of the components under a static electric field, which was confirmed by nitrogen surface enrichment measurements. This surface modification technique introduced insight into multicomponent electrospinning and leads to a promising perspective for the production of surface-biofunctionalized nanofibers.

Improving Gas Barrier Properties of Recycled PET

Richard J. Spontak and Jan Genzer
United Resource Recovery Corporation
$250,000
2006 to 2011

We are aiming to decrease the permeation of gases through recycled poly(ethylene terephthalate) (PET) by incorporating nanoclays to modify the recycled PET surface. Attachment of single clay platelets on chemically-modified PET surfaces will yield exfoliated polymer-clay nanocomposites after extrusion. This bottom-up approach eliminates the requirement of using organically-modified clays, which causes degradation of the PET matrix at high extrusion temperatures. In addition, we are also studying the formation of silica-like layers on PET by exposing silicon-coated PET sheets to UV-ozone treatment, which yields functionalized PET surfaces and reduces permeation of gases.

Triblock Copolymer Gels as Fabric Sensors and Actuators

Tushar K. Ghosh and Richard J. Spontak
National Science Foundation
$368,000
2007 to 2010

Thermoplastic elastomer gels of triblock copolymers modified by a midblock-selective solvent show potential as electroactive polymers for the design of resilient, lightweight and efficient actuators. The proposed research aims to elucidate the effect of polymer morphology, composition and chemistry on electroactivity. While materials used in previous studies were styrenic block copolymers with diene midblocks, this approach focuses on acrylate triblock copolymers and terpolymers, which are compatible with polar solvents, increasing the dielectric constant and reducing the electric field required for actuation. This development overcomes a major hurdle in the practical application of these actuators.

Multicomponent Electrospun Polymer Nano/Microfibers

Richard J. Spontak
National Science Foundation Graduate Fellowship
$102,000
2007 to 2010

Electrospinning is an ideal way to create new materials that can be fashioned into nonwovens for commercial applications. In this work, we are examining novel polymer blends and nanocomposites wherein mixing and/or dispersion constitute important property-development considerations. In one instance, Bombyx mori silk and poly(glycolic acid-co-lactic acid) have been blended and electrospun to create tissue scaffolds. Silk has good mechanical properties but poor degradation and biocompatibility, while PGLA has a fast degradation time and excellent compatibility. The target tissue in this investigation is ligament or tendon, which must have equivalently high moduli and tensile strength.

Interfacial Modification of Polymer/Polymer Thin Films

Richard J. Spontak
National Science Foundation
$109,000
2008 to 2009

A guest macromolecule, consisting of either a block copolymer (BCP) or a core-shell microgel (MG) particle, has been used to stabilize a molecularly thin polymer film positioned atop a substrate of a chemically-incompatible polymer substrate. Modification of the polymer/polymer interface due to interfacial partitioning of the guest macromolecule significantly increases the stability of the top film by either slowing down or completely eliminating dewetting. It has been established that the dewetting rate of the top film depends on (i) the concentration of guest macromolecule, (ii) the film thickness and (iii) the annealing temperature.

Colloidal and Biocolloidal Engineering on Electrically Controlled Microchips: New Principles for Making Bionanomaterials, Microbioassys and Microrobots.

Camille Dreyfus Teacher-Scholar Award
PI: Orlin Velev
$ 75,000
06/2006 to 05/2011

We are developing new microfluidic microchips that will be used to assemble new materials, fabricate biological microstructures and nanocomposites, ultimately leading to autonomous devices such as microrobots. We will use DEP techniques for the assembly of biocomposites from cells and protein-functionalized nanoparticles that will serve as "biocolloidal glue" for the cells. These bionanomaterials will combine the functionality of the cells and the particles and could be used in biosensors, microbioreactors and microsurgery. We will also develop motile "smart" particles based on semiconductor chips that can be used for biological and materials manipulation on the microscale.

NIRT: Nanoscale Directed Self-Assembly in Electrical and Optical Fields

Co-PI(s): Norman Wagner, Orlin Velev, Eric Furst, John Brady and Eric Kaler
National Science Foundation
$ 1,335,000 (total), $ 224,000 (Velev NCSU subcontract)
07/2005 to 06/2009

University of Delaware, North Carolina State University and California Institute of Technology

Engineering micro-to-nanoscale devices and nanostructured materials requires control and understanding of the thermodynamics and dynamics of self-assembly of nanoscale - building blocks in solution. This process is hierarchical in nature, so that molecular-level physics and chemistry lead to interaction potentials between nanoparticles and solvent molecules, which under the action of external fields can assemble into higher-order structures on the nano-to-micron scale with emergent functionality. We propose an integrated scientific and educational program to develop novel routes using directed self-assembly to manufacture nanoscale devices and advance the state of knowledge in the field of nanoscale manufacturing.

NIRT: Engineered Molecular Fluidics

National Science Foundation
PI(s): Sergei Sheiko, Michael Rubinstein, Orlin Velev, Krzysztof Matyjaszewski
$ 1,160,000 (total), $ 274,000 (Velev NCSU subcontract)
09/2006 to 08/2010
University of North Carolina - Chapel Hill, North Carolina State University and Carnegie Mellon University

We are developing a new area of engineered molecular fluidics, which involves synthetic design of flow-responsive molecules, experimental and theoretical studies of surface-confined macromolecules under flow, and the engineering of flow actuation techniques. Experimental findings will be continuously tested against theoretical predictions and computer simulation studies. The group of Velev is working on actuation principles and techniques for manipulation of fluid monolayers on solid substrates by using electric fields. These techniques will be applied to pattern polymer monolayers and transfer the patterns on various surfaces, creating materials with surfaces that may be ultrahydrophobic, anisotropically wetted or directionally conductive.

CAREER: Colloidal Assembly and Transport Using Dielectrophoresis and Novel Media

Orlin D. Velev
National Science Foundation
$405,000
03/2003 to 08/2009

New microstructured materials and devices from colloidal components will be designed and assembled in a manner similar to the present design of electrical microcircuits. Three new techniques will be developed: (1) dielectrophoretic manipulation of colloidal particles in on-chip structures with electrical and photonic functionality, (2) transporting and manipulating droplets and particles suspended in a new type of liquid substrate chip, and (3) use of liquid CO_2 as a new medium for controllable colloidal assembly. The integrated educational projects will introduce the principles of nanoscale engineering into such disciplines as chemical and electrical engineering, materials science, and applied physics.

International supplement to CAREER: Colloidal assembly and transport using dielectrophoresis and novel media

Orlin D. Velev
National Science Foundation
$25,800
03/2003 to 08/2009

The international supplement to the CAREER award supports a research collaboration aimed at developing techniques for the synthesis of a new class of particles, which will be assembled into a variety of smart gels, photonic crystals, colloidal liquid crystals and others. The collaboration involves two groups, one in US (of the PI O. Velev) and one in UK (of the collaborator V. Paunov). The supplement allows meetings between the collaborators, organization of joint workshops and hosting of a UK graduate student or postdoctoral fellow for a long-term research experience.

Development of Highly Functional Materials for Packaging and Liquid Delivery Based on Embedded Microfluidic Networks and Nanomaterials

Orlin D. Velev
MeadWestvaco Research Center
$ 270,000
10/01/2007 to 09/30/2010

This project will develop a new class of highly functional materials with embedded microfluidic networks and nanomaterials. These materials will be inspired by the rich functionality of natural skin derived from its vesicular blood "microfluidic" networks. We propose to design and test new materials and products such as flexible sheets that can be solidified on demand to yield specific shapes, patches that can eject liquid droplets by mechanical actuation, polymer skins that release antimicrobial agents on touch and films with very high heat exchange efficiency.

New Generation of Lab on Chip Separators based on Independent Fluid and Analyte Control

PIs: Dimiter Petsev, Univ. of New Mexico, Orlin Velev, NCSU, Steven Cramer, RPI
National Science Foundation
$ 417,590 ($ 171,463 NCSU Velev subcontract),
08/31/2008 to 07/31/2011

The objective of this project is to develop a novel method for the separation and sensing of biomolecules by decoupling the electroosmotic transport of the fluid from the electrophoretic migration of the solutes. This will be accomplished by means of new elements which we developed recently - semiconductor diode pumps powered by an AC field. The analytes will be independently manipulated electrophoretically by a direct current (DC). We will also explore the fabrication and properties of a new class of microscopic device-like particles that can move, sense and respond to biochemical stimuli on their own.

Organic-Inorganic Colloidal Particles: Physical Properties and Applications in Food and Emulsions

Orlin D. Velev
Unilever R&D, Vlaardingen, Holland
$ 92,478
09/01/2008 to 08/31/2009

The NCSU investigator is collaborating with Unilever R&D – Vlaardingen on the synthesis, characterization and application of colloidal organic-inorganic particles. These core-shell particles can bring dual functionality to consumer products – they can stabilize foams and emulsions by virtue of their hydrophobic coating and they can deliver food micronutrients through their inorganic core. The research team at NCSU is developing new particles and is focusing on their physical properties, wetting and adsorption behavior and use as stabilizers of foams, emulsions, thin films and gels.

Novel Types of Flexible Photovoltaic Cells Based on Aqueous Gels and Ionic Rectifying Junctions

Orlin D. Velev
Air Force Research Laboratory/ AT&T Government Solutions
PI: Orlin Velev
$ 60,000
10/01/2008 to 08/31/2009

This exploratory project will test a transforming concept in the area of organic photovoltaic cells. We will create a new generation of cells that will operate on the basis of water-based polyelectrolyte-doped gels. By doping the gel diodes with ionic photosensitive molecules we create solar cells where the doped gels will separate the charges and generate current through the electrodes. These light harvesting devices have the potential to be extremely inexpensive, flexible, scalable and environmentally friendly. This project will provide proof of concept, evaluation of prototype performance and directions for future development of the new technology.

Nanostructured Materials for Renewable Alternative Energy

Gregory Parsons, Orlin Velev, Michael Dickey, Veena Misra, Christopher Gorman
US Department of Energy
$ 625,916 ($ 77,273 Velev part)
07/25/2008 to 07/24/2009

The objective of this program is to achieve improvements in solar absorptivity and energy transduction in organic photovoltaic devices and to obtaining a detailed understanding of the fundamental relations between nanoscale structure and chemical composition for improving PV and other renewable energy systems. For example, new nanoscale patterning, self-assembly, and atomic-scale thin film coating techniques are being developed that can produce new high surface area inorganic and organic/inorganic hybrid materials systems useful for PV and other energy transduction platforms.

New Principles for Interfacial Engineering and Superstabilization of Biphase Systems by Using Particles with Engineered Structure and Properties

Orlin D. Velev
U.S. Army Research Office
$ 387,000
06/01/2009 to 05/31/2013

New types of interfacially-active particles will be synthesized and will be used to make surfaces with extraordinary properties and foams and emulsions with extraordinary stability. The project includes three components: (1) Synthesis of new classes of particles with engineered properties. (2) Designing of interfaces with extraordinary strong adsorption layers. (3) Investigation of realistic foams and emulsions stabilized with advanced particles. The new types of superstable foams and emulsions developed in the project could be used in WMD decontamination or shielding formulations with improved functionality, stability and ability to provide visual warning.

CHEMICAL ENGINEERING FACULTY

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