

## Chemical and Biomolecular Engineering research projects 2006-07

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### 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](http://www.nsfstc.unc.edu).

### A Systematic Approach Towards the Detection of Bioterrorism Agents in Complex Sample Matrices

*Ruben G. Carbonell and Lee-Ann Jaykus  
National Center for Food Protection and Defense  
\$236,000  
2006-2007*

This is the first phase of a study aimed at the development of inexpensive, robust ligands for the capture and detection of B. anthracis spores and Ricin toxin in complex mixtures. After ligand identification using combinatorial peptide and aptamer libraries, additional funds will be requested to develop novel capture media and detection strategies.

### A Systematic Approach toward the Quantitative Determination of Pathogen Load in Complex Sample Matrices

*Ruben G. Carbonell and Lee-Ann Jaykus  
Food Safety Research and Response Network – USDA  
\$55,000  
2006-2007*

This project aims at the development of novel, robust and inexpensive ligands for the capture and detection of Salmonella in food products. This is an initial exploratory grant to identify ligands by solid phase combinatorial peptide libraries and aptamer libraries. In future phases of the work the focus will be on device development for capture, detection and analysis.

### 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.

### Development of CO<sub>2</sub>-Based Deposition Techniques for Production of Tunable Coatings on the Surfaces of Elastomers

*Jan Genzer  
Kenan Center for the Utilization of Carbon Dioxide in Manufacturing, NCSU  
\$28,500  
11/1/06 to 10/31/2007*

The major theme of this project is to develop techniques for attaching semifluorinated organic modifiers from supercritical CO<sub>2</sub> 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 1/31/2009*

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 6/30/2007

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, Purdue)

NSF-NIRT

\$1,700,000 (\$417,499 for J. Genzer)

7/1/2004 to 6/30/2008

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 Liebmman-Vinson

(co-PI, BDT)

ONR

\$1,193,000 (\$460,899 for J. Genzer)

1/1/2005-12/31/2007

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.

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

Christine S. Grant

National Science Foundation: GOALI

\$270,000

2004-2007

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.

### **NCSU/NCA&T Program for STEM Enrollment Enhancement**

*John Fountain, Joel Ducoste, Christine S. Grant and others*

*National Science Foundation*

*\$350,016*

*1/03 to 12/06*

NCSU and NCA&T are developing a program to increase the number of graduates in science, technology, engineering and mathematics (STEM). Program elements include: NCSU summer camp for graduating high school students; summer bridge programs at both schools to prepare new students for introductory college science and math courses; undergraduate research programs, tutoring; mentoring of STEM majors; and faculty exchange between the two campuses. Comprehensive monitoring will provide data to evaluate each program element. Success in the program will result in an increase in the number of STEM graduates, through both an increase in the number and retention of entering majors.

### **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 is focused on improved recruitment and retention by addressing unique issues at the intersection of race and gender, leading a series of “summits and mini-summits”. The goals are to identify best practices for successful recruitment, retention and promotion and create a peer mentoring network for WOC in engineering academia.

### **Underrepresented Engineering Faculty Peer Mentoring Workshop and Mini-Summits (PAESMEM)**

*Christine S. Grant*

*National Science Foundation*

*\$28,000*

*9/05 – 7/07*

The goal is to lead a series of faculty/administrator workshops/mini-summits in conjunction with the National Academy of Engineering’s Center for the Advancement of Scholarship on Engineering Education (CASEE). The workshops’ intent is to develop an action plan for Grant’s “Promoting Under Represented Presence On Science and Engineering faculty (PURPOSE) Institute”. Key aspects include: (1) Identification of obstacles to the recruitment/retention of minority engineering faculty. (2) Identification of critical needs for an interdisciplinary, multicultural faculty peer mentoring network. (3) Building effective faculty networks and initiating the creation of a roadmap for institutional change. Presentations of outcomes disseminated to Engineering Deans at ASEE meetings.

### **PURPOSE\* Institute Faculty Leadership Program: A University Extension, Engagement, and Economic Development Grant (\*Promoting Under Represented Presence On Science and Engineering Faculty)**

*Christine S. Grant*

*NCSU University Extension Grant Program*

*\$13,000 (\$6500 – VC Extension; \$6500 – COE Match)*

*7/05 – 6/06*

The primary goal of the PURPOSE Institute is to Empower Current and Aspiring Faculty to Achievement, Promotion and Leadership in the Academy. The Institute represents a focused effort to diversify science and engineering faculties. Institute initiatives address the leadership development of the same engineering faculty in their respective fields, at their home institution and in the university system as a whole. Certain aspects of the faculty/administrator partnerships may be integrated into both university practices, and existing efforts in the UNC system, providing institutional leadership with a roadmap for the recruiting, promotion and retention of diverse engineering faculty members.

### **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 – 12/09*

This REU award for a 3 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.

### **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*

*2005-08*

LANGURE’s ultimate aim is to institutionalize the teaching of research ethics. It is 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 jointly 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.

### **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.

### **NSF/NIRT. Surfactant Self-Assembly on Nano-Structured Surfaces: Multi-Scale Computational Prediction and Design**

*Keith E. Gubbins*

*National Science Foundation*

*\$1,300,000*

*09/01/04-08/31/08*

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).

### **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 01/31/08*

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.

### **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.

### **U.S.-Poland Workshop on Nanoscience and Nano-Structured Materials**

*Keith E. Gubbins*

*NSF*

*\$31,393*

*06/01/2006 to 11/30/2006*

This provides support for the US participants in the First US-Poland Workshop on Nanoscience and Nano-Structured Materials, held in Poznan, Poland from June 26 to 28, 2006. The US organizers are K.E. Gubbins and M. Radosz (University of Wyoming). The Workshop had 12 invited speakers from the U.S., and 12 from Poland, and its aim is to make both sides familiar with research being done in the partner country, and to encourage future contacts and research collaboration.

### **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*

*\$91,400*

*07/01/2007 – 06/30/2010*

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.

### **Computer Simulation Studies of Protein Aggregation**

*National Institutes of Health*

*Carol Hall*

*\$813,524*

*12/1/04 -11/30/08*

The aberrant assembly of normally soluble proteins into ordered aggregates, called amyloid fibrils, is a cause or associated symptom of many different human disorders including Alzheimer's and Parkinson's diseases. 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 fibril formation by using discontinuous molecular dynamics to simulate multi-protein systems containing polyalanine chains modeled using our intermediate-resolution model, PRIME, (2) to shed light on the molecular-level mechanisms responsible for the aggregation of polyglutamine, the protein whose fibrillization is linked to Huntington's disease, and (3) to investigate the aggregation and possible fibrillization of multi-protein systems containing specific amyloidogenic peptides by extending PRIME to a coarse-grained representation of all 20 residues.

### **PECASE: Intracellular Signaling Networks in the Immune Response**

*Jason Haugh*

*NSF-Bioengineering & Environmental Systems, #0133594*

*\$375,000*

*2/15/02 - 7/31/07*

This five-year study seeks to characterize crosstalk among signal transduction pathways stimulated by IL-2 and IL-4 in T cells, using quantitative biochemical measurements and mathematical modeling. Educational objectives include integration of molecular immunology in graduate and undergraduate courses as well as in K-12 outreach.

### **Molecular Crosstalk in Intracellular Signaling Networks**

*Jason Haugh*

*NIH-General Medical Sciences, R01-GM067739*

*\$710,180*

*9/1/03 - 8/31/07*

In this four-year 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 - 5/15/08*

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.

### **Integration of Soluble and Adhesive Gradient Signals in Directed Cell Migration**

Jason Haugh  
ONR-Young Investigator Program, N00014-03-1-0594  
\$299,898  
6/1/03 - 11/30/06

The goals of this three-year project are to image and model PI 3-kinase activation and biophysical aspects of fibroblast motility in response to gradients of both soluble PDGF and immobilized fibronectin, with implications for influencing tissue repair.

### **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.

### **The Role of Asphaltenes, Naphthenates and Other Surface-Active Molecules in Colloidal Aggregate Formation and in Water-In-Oil Emulsion Stabilization**

Peter K. Kilpatrick  
Industrial Consortium (Nalco Chemical, Energy Services Division; ConocoPhillips; ExxonMobil, Shell Exploration and Production Company, Champion Technologies)  
\$950,000  
6/16/00 to 6/15/07

Asphaltenes, resins, and the solvency of the crude are known to play significant roles in the stabilization of water-in-crude oil emulsions. What is considerably less well understood are the roles of naphthenic acids (or naphthenates) and of asphaltene incompatibility due to blending on emulsion stability. In this industrially sponsored consortium project, we are studying model and whole petroleum naphthenates

and blends utilizing the methods of critical electric field, interface rheology, and the centrifugation technique. Naphthenates stabilize emulsions through a liquid crystal mechanism while asphaltenes stabilize through an elastic film mechanism.

### **Biotransformations Near and Above 100°C: Mining hyperthermophile genomes for novel biocatalysts**

Robert M. Kelly and Michael W.W. Adams (Univ. of Georgia)  
National Science Foundation  
\$400,000 (RMK)  
9/1/03 to 8/31/07

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 scientific and technological importance.

### **Polypeptide and Polysaccharide Processing by Heterotrophic Hyperthermophilic Microorganisms**

Robert M. Kelly  
Department of Energy  
\$362,380  
8/1/03 to 7/31/07

This project focuses on the physiological, biochemical and genetic characterization of heterotrophic hyperthermophilic microorganisms with respect to mechanisms by which these organisms process polypeptides and polysaccharides under normal and stressed conditions. Targeted and whole genome cDNA microarrays will be used to track differential expression of known and putative genes related to proteolysis, glycoside hydrolysis, sugar and peptide transport, stress response and compatible solute formation. This project continues efforts to understand ecological and physiological aspects of hyperthermophiles as they relate to their high temperature habitats.

### **Microbial Ecology in High Temperature Biotopes**

Robert M. Kelly  
NASA  
\$391,000  
5/1/03 to 4/30/07

Microbial ecology of hyperthermophiles is studied with emphasis on how these microorganisms colonize thermal niches and interact in mixed communities. A functional genomics approach is used, in conjunction with biochemical and microbiological characterization of features revealed through differential gene expression. Hyperthermophiles are examined individually and in mixed cultures for physiological characteristics that relate to: physical, chemical and biological aspects of their growth environment, inter- and intra-species interactions, propensity for forming biofilms, and existence of a naturally competent state for gene transfer. These issues are central to understand the evolution of terrestrial life and to extraterrestrial exploration of microbiological phenomena.

### Graduate Training in Biotechnology

*Robert M. Kelly, PI + 30 other NCSU faculty*  
*National Institutes of Health*  
 \$1,200,000  
 7/1/05 to 6/30/10

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*  
 \$304,186  
 8/15/03 to 8/14/07

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.

### Investigation of Potential Genes for the Production of Glucose Binding Proteins

*Robert M. Kelly*  
*BD Technologies, Inc.*  
 \$25,000  
 8/1/05 to 7/31/06

The potential for selected carbohydrate binding proteins encoded in the genomes of hyperthermophilic microorganisms were investigated for their potential use in glucose sensors.

### Purification of 2u-Globulin

*Robert M. Kelly*  
*Integrated Laboratory Systems, Inc.*  
 \$20,500  
 6/1/06 – 12/31/06

Rat 2u-globulin (18.7 kDa) is a member of a group of proteins known as the lipocalins, which are believed to function in the binding and transport of small, lipophilic molecules, and include retinol-binding protein and apolipoprotein D. This project focuses on the purification and characterization of Rat 2u-globulin in support of efforts at ILS to validate an ELISA to quantify levels of this protein in kidney homogenates to determine the mode of action of chemicals demonstrated to induce renal tumors in male rats.

### Functional genomics screening for novel glycosyl hydrolases in the extremely thermophilic bacterium *Caldicellulosiruptor saccharolyticus* using a targeted DNA microarray

*Robert M. Kelly*  
*Genencor International, Inc.*  
 \$12,500  
 6/1/06 to 5/31/07

The DOE Joint Genomes Institute (JGI) is currently completing the genome sequence of the H<sub>2</sub>-producing extremely thermophilic bacterium *Caldicellulosiruptor saccharolyticus* through a project initiated by an international hydrogenomics

consortium, which includes Genencor International, Wageningen University (The Netherlands) and North Carolina State University. As part of this effort, 500-ORF, targeted DNA oligonucleotide microarray is being developed to examine the transcriptional response of *C. saccharolyticus* on a variety of carbohydrate substrates to identify novel glycosyl hydrolases that are potentially useful in for biohydrogen production.

### Biotransformations Near and Above 100°C: Bioenergy conversion using hyperthermophilic microorganisms and enzymes

*Robert M. Kelly and Michael W.W. Adams (Univ. of Georgia)*  
*National Science Foundation*  
 \$440,000 (RMK)  
 9/1/06 to 8/31/09

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 and microorganisms for bioenergy conversion.

### Functional Nanofibers from Associative Polymers through Electrospinning

*Nonwoven Cooperative Research Center (NCRC)*  
*Saad A. Khan, Juan Hinestroza and Benham Pourdeyhimi*  
 \$150,000 (direct cost)  
 7/05-7/08

The proposal aims at developing novel functional nanofibers using new generation associative polymers with potential applications in surface modification of nonwoven fabric. Hydrophobically-modified alkali soluble emulsion (HASE) polymers form an interesting class of associative polymers as they possess a negatively charged polymeric backbone with pendant hydrophobes. The hydrophobicity and electrostatic charge of these polymers can be controlled in solution and the rheological properties of these solutions can be modulated. Furthermore the properties of these polymers can be altered to suit a particular application by embedding application-specific functional moieties.

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

*Nonwoven Cooperative Research Center (NCRC)*  
*Saad Khan\* and Benham Pourdeyhimi*  
 \$120,000 (direct cost)  
 7/06-7/09

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

9/06-9/09

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 nanofibrillar 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 Research Center (NCRC)*

*Russel Gorga, Don Shiffler and Saad A. Khan*

\$120,000 (direct cost)

1/07-7/10

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.

### **Source-based Pollution Prevention through Depolymerization of Polyethylene Terephthalate (PET) in Supercritical CO<sub>2</sub>**

*National Science Foundation*

*George Roberts and Saad Khan*

\$361,679

12/01-12/07

We present an exciting new approach to pollution prevention at the source through elimination of waste (off-specification, unusable polymer) that is generated during the production of Poly(ethylene terephthalate) (PET). We propose to investigate a single-step, extrusion-based process to depolymerize PET and recover purified monomeric and oligomeric units for repolymerization. The two key features to the novel process are the: 1) use of a twin-screw extruder to convey the polymer and to continuously create the fresh surface area that is required for the depolymerizing agent to penetrate into the polymer; and, 2) use of supercritical carbon dioxide as a processing aid.

### **Electrospinning of Polymer Melts**

*NSF S&T Center*

*Saad Khan*

\$120,000; 8/06-8/08

Conventional electrospinning is a solvent intensive process. In this project, we develop a new strategy to electrospin fibers directly from the melt state. The effects of process variables and material properties on the characteristics of the melt electrospun fibers will be examined.

### **Evaluation of Fast Clad Urethane Paint System for Three Bridges Over US 64 in**

*Wake County, North Carolina*

*P. K. Lim*

*NC Department of Transportation*

8/1/05-7/31/07

\$49,280

The project will evaluate the cost effectiveness of a new, two-coat paint system—as represented by Sherwin-Williams Fast Clad Organic Zinc/Urethane system—on three overpass bridges and to compare the cost effectiveness of the new paint system with that of standard three-coat paint system that has been used by NC Department of Transportation for many years and that will also be evaluated on three other overpass bridges. The project will make recommendations on the advisability of replacing the standard three-coat paint system with the new, two-coat paint system.

### **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

1/06–12/08

Glycerol is a byproduct of biodiesel synthesis from the tri-glycerides 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. 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.

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

*H. Henry Lamb*

*Novozymes*

\$25,000

2/07-1/08

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 will investigate the simultaneous enzymatic hydrolysis of corn starch and fermentation of the resulting glucose to ethanol by yeast (*Saccharomyces cerevisiae*). The goal will be to optimize the batch process to achieve maximum ethanol productivity while making efficient use of added  $\alpha$ -amylase and glucoamylase enzymes. This project will involve detailed mathematical modeling using laboratory kinetics data on enzymatic liquefaction and saccharification and yeast growth kinetics on glucose to predict ethanol productivity and yield.

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

*D.F. Ollis*

*NSF*

*8/1/04-7/31/08*

*\$300,000. (NSF DTS Award)*

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

### Dielectric and Gate Electrode Materials for Advanced Electronic Devices

### Metal Film Materials Deposition from Supercritical CO<sub>2</sub>

*Gregory Parsons*

*NSF Science and Technology Center for Environmentally Responsible Solvents and Processes*

*\$130,000*

*11/01/04 to 10/31/06*

Future integrated circuits and devices will likely require new lower temperature chemical processing approaches. Through the NSF Science and Technology Center at NC State, we are studying the application of supercritical CO<sub>2</sub> as a potential solvent in advanced deposition approaches for metal and metal oxide materials. We are specifically evaluating the application of solvation forces to supply energy to deposition surface reactions, to enable high quality dielectric and metal thin films to be formed at low deposition temperatures.

### Hierarchical Assembly of Interconnects for Molecules Electronics

*Chris Gorman (PI, NCSU Chemistry) Gregory Parsons*

*(co-PI) and Dan Feldheim (co-PI, NCSU Chemistry)*

*NSF- NIRT*

*\$1,160,000*

*08/15/2003 through 07/31/2007*

Characterization of molecules and molecule-scale constructs requires chemical processes to reliably control nanometer-scale interconnect structures. For this NSF-NIRT project, our group is focusing on techniques to build and test molecular-scale characterization test-beds. This includes nanoscale patterning by nano-imprint lithography and edge-defined lithography, as well as analysis of charge transport in molecular systems. We collaborate closely with professors Gorman and Feldheim in Chemistry at NC State in the area of molecular synthesis and assembly.

### Porphyrim-Based Photovoltaics

*Gregory Parsons*

*SolarAmp Inc.*

*\$163,000*

*02/01/2004 through 8/31/2006*

The ability to generate clean energy at low cost will have significant positive impact in many areas. In our work, we are collaborating with the Lindsey group in Chemistry at NC State to construct and characterize porphyrin molecule-based solid state photovoltaic cells to test these materials as potential future low-cost alternatives to inorganic semiconductors in direct solar energy conversion devices. Our device utilizes a molecular-assembled porphyrin photo-antenna approach that differentiates it from other organic photovoltaic device structures.

### Design of catalytic carbon nano-materials for enhanced H<sub>2</sub> production from thermal water splitting

*Marco Buongiorno Nardelli (PI, NCSU Physics), Gregory Parsons (co-PI), Tom Pearl (co-PI, NCSU Physics)*

*NCSU Nanotechnology Steering Committee*

*\$50,000*

*9/1/2005–8/31/2006*

A necessary step towards the achievement of a hydrogen-based economy is the development of a production process that is able to drastically revamp the energetic cost while leaving, at the same time, a smaller environmental footprint than the current industry standards. Hydrogen is a constituent of water, and if viable extraction processes could be found, we would have an endless reservoir of clean fuel all around us. This project is a combined theoretical/experimental study to gain a fundamental understanding of the factors that influence reaction mechanism, rate and yield for H<sub>2</sub> producing reactions carried out in nano-structured carbon-based materials. We aim to profit from such fundamental knowledge by designing nano-catalyst systems to achieve a breakthrough in H<sub>2</sub> production.

### Smart Textiles via Self-Assembled Nanolayers and Atomic Layer Deposition

*Gregory Parsons (co-PI) Juan Hinestroza (co-PI, Cornell Univ.)*

*NCSU Nanotechnology Steering Committee*

*\$50,000*

*9/1/2005–8/31/2006*

This multidisciplinary proposal aims at using, for the first time, atomic layer deposition and self-assembled nanolayers to selectively customize the surface of textiles substrates. Due to the high curvature and viscoelastic nature of textile fibers existing technologies are not able to provide full coverage of a fiber's surface. The use of self-assembly techniques and self-limiting reactant adsorption processes offer the possibility of achieving fully conformal functionalization of textile fibers of any continuous shape. The ability to control the composition of the surface at the molecular level opens the possibility of developing smart textiles for applications such as active filtration, bioseparation of proteins, catalytic mantles, electronic fabrics as well as novel barrier and anticounterfeiting materials.

### Approach for Integration of Ballistic Interconnect Materials

*Gregory Parsons (PI)*

*Semiconductor Research Corporation*

*\$40,000*

*Jan 1, 2006 – Dec 31, 2007*

Interconnect technology has reached a scaling limit where the impact on system performance from surface roughness and scattering effects in conventional copper interconnects is significant. Alternative materials and processing technologies that offer improved scaling performance must be identified. Candidate interconnect technologies require very large electronic conductivity at extremely scaled dimensions. Carbon nanotubes which support current densities well in excess of the 2013 International Technology Roadmap for Semiconductors value of  $3.3 \times 10^6$  A/cm<sup>2</sup>. For this effort, we will demonstrate a method for synthesizing and aligning nanotube bundles and selectively coating these bundles

with metals in the contact structures to achieve integrated high performance interconnects compatible with further processing.

### **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– 12/08

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  
 4/07– 4/09

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.

### **Continuous Polymerization in Supercritical Carbon Dioxide**

*George W. Roberts*  
*Kenan Center for the Utilization of Carbon Dioxide in Manufacturing*  
 \$300,000  
 10/01/97 – 05/15/07

Free-radical, chain-growth polymerization in supercritical carbon dioxide is being investigated in a continuous, stirred-autoclave reactor. Current emphasis is on the polymerization of acrylic acid. Models of the polymerization process are being developed. The decomposition kinetics of various initiators also were studied in supercritical carbon dioxide.

### **Selective Catalytic Hydrogenation of Aromatic Polymers Facilitated by Supercritical Carbon Dioxide**

*George W. Roberts*  
*Army Research Office*  
 \$343,183  
 07/01/01 – 06/30/06

The objective of this research is to develop catalytic process technology for the selective hydrogenation of aromatic polymers. Supercritical carbon dioxide will be used as a processing aid in order to reduce the viscosity of the polymer solution that is being hydrogenated. The initial thrust of the research is to identify solvents that have a high solubility for polystyrene, and are compatible with supercritical CO<sub>2</sub>, such that the polymer does not precipitate at high CO<sub>2</sub> partial pressures

### **Homogeneous Co-polymerization of Fluoromonomers in Supercritical Carbon Dioxide**

*George W. Roberts*  
*National Science Foundation Center for Environmentally Responsible Solvents and Processes*  
 \$150,000  
 10/01/03 – 10/31/06

Free-radical, chain-growth co-polymerization of vinylidene fluoride and hexafluoropropylene in supercritical carbon dioxide is being investigated in a batch reactor and in a continuous, stirred-autoclave reactor. Models of the polymerization process are being developed.

### **Source-Based Pollution Prevention through Depolymerization of Poly(ethylene terephthalate) with Supercritical Carbon Dioxide**

*George W. Roberts (Saad A. Khan, co-PI)*  
*National Science Foundation*  
 \$361,679  
 12/15/01 – 11/30/06

A single-step, extrusion-based process to depolymerize poly(ethylene terephthalate) and recover purified monomeric and oligimeric units for repolymerization is being investigated. Two key features of this technology are: 1) a twin-screw extruder is used as a reactor to convey the polymer and to create the fresh surface area that is required for the depolymerizing agent, methanol of ethylene glycol, to penetrate into the polymer, and; 2) supercritical carbon dioxide is used as a processing aid.

### **Synthesis of Superabsorbent Polymers in Supercritical Carbon Dioxide**

*George W. Roberts*  
*Stockhausen, Inc. (Greensboro, NC)*  
 \$236,515  
 04/01/05 – 03/31/07

The objective of this program is to learn how to produce a cross-linked, partially neutralized poly(acrylic acid) polymer that has superior properties for use as a superabsorbent polymer, using supercritical carbon dioxide as the reaction medium.

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

*Camille Dreyfus Teacher-Scholar Award*

*PI: Orlin Velev*

*\$75,000, Period covered: 06/2006 - 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 - 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 - 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 - 02/2008*

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<sub>2</sub> 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 - 02/2008*

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.

### **Capillarity-Driven Deposition of Functional Biomolecular Nanocoatings and Nanopatterns**

*Air Force Office of Scientific Research (AFOSR)*

*PI: Orlin Velev*

*\$118,000*

*08/2006 - 07/2007*

We are developing techniques that will allow rapid, scalable and engineered deposition of functional bio-derived coatings and wires. The project is based on the method for convective and shear-driven deposition of nanofilms developed in the group of Velev, combined with the extensive experience in biological and biologically-inspired nanomaterials at the AFRL. We will also develop a new technique for the deposition of the virus and nanoparticle wires in precise patterns by moving a capillary and assembling biomaterials in its trailing meniscus. These precisely deposited single bioscaffold wires will allow fabrication of biomolecule-derived on chip sensors and electronic devices.

### **STIR - Development and Evaluation of Realistic Microbioassays in Droplets on a Chip**

*Army Research Office*

*PI: Orlin Velev*

*\$50,000*

*10/01/2006 – 06/30/2007*

The new dielectrophoretic droplet chips developed in the group of Velev will be used in microscopic bioassays based on agglutination of antibody-conjugated particles. This project will evaluate the limit of detection of the assays and will seek ways to minimize the time required for result readout. The experiments will be interpreted by modeling the kinetics of particle agglutination and mass transfer processes inside the droplets. The study will be performed with antibodies and antigens supplied by the DOD Critical Reagents Program and the performance of the microbioassays will be compared to the standard Army assays.

### **NER: Large-scale synthesis and assembly of micro- and nanoparticles with dipolar charge and anisotropic shape**

*Orlin D. Velev*  
National Science Foundation  
\$114,000  
08/2004 - 07/2006

This project will for the first time allow the large-scale, efficient and inexpensive fabrication of colloidal particles with anisotropic shape and/or directional interactions. The first class of novel particles that will be fabricated will have permanent dipolar and/or quadrupolar moments. The second type of new particles is cylindrical polymer microrods. We have discovered a scalable process for making such microrods by shearing and “drying” of emulsified droplets from polymer solution. These anisotropic particles will be used for the assembly of advanced materials such as ion- and pH-sensitive gels, colloidal liquid crystals, photonic crystals and electrorheological fluids.

### **Microstructure and functionality of processed cheese: the role of milkfat**

*PI: Christopher Daubert, Co-PIs: Richard Hartel and Orlin Velev*  
Dairy Management Inc. (DMI)  
\$218,617  
01/2005 - 12/2007  
North Carolina State University and University of Wisconsin

An understanding of how cooling schedules affect processed cheese and other foods with casein gel-based microstructure (spreads and yogurts) may lead to more efficient cooling rates during the final phase of product manufacturing. Cooling schemes have been shown to directly impact processed cheese functional attributes, specifically melt and shred. Understanding how cooling conditions influence food nanostructure: protein gelation, fat crystallization, and their interactions could lead to shortened cooling times and increased refrigeration throughput, while producing higher quality products.

### **New Principles for Nanofluidics and Microencapsulation Based on Polymer Phase Separations and Electric Field Manipulation.**

*PI: Orlin Velev*  
Phillip Morris USA/Quantum Resources Corp.  
\$25,000 + \$80,000 Visiting researcher fellowship  
01/2006 – 12/2007

We are developing novel complex microfluidic devices, microscopic “smart” capsules and new functional nanomaterials. First, we use coaxially spun nanofibers as channels and separators in new class of nanofluidic devices. These devices

could be used for analysis of extremely small volumes of biological molecules or chemical agents. Second, we are developing new types of polymer capsules that could be manipulated by magnetic or electric fields and triggered by UV light, pH, temperature, pressure gradients, microwaves or magnetic fields. These projects are developed within the Interdisciplinary Network of Emerging Science & Technologies of PM – USA.

### **Evaluation of the Potential of Rod-Like Particles Made of Modified Cellulose as Superstabilizers of Industrial Emulsions and Suspoemulsions**

*DuPont (Engineering grant)*  
*PI: Orlin Velev*  
\$15,000  
08/2006 - 07/2007

We are investigating and evaluating a new class of foam and emulsion stabilizers, based on nano- and microparticles from polymers and hydrophobically modified cellulose. This will allow replacing the synthetic molecular surfactants with nanoparticles derived from inexpensive polymers or cellulose, an abundant natural product. This proposal is based on a new process for making rod-like polymer particles by shear and solvent attrition that has been recently developed by Velev and collaborators at NCSU. These rod-like particles produce “superstabilized” foams and emulsions that have vastly superior resistance to breakdown than their common surfactant-based analogues.

## **CHEMICAL ENGINEERING FACULTY**

**Lisa G. Bullard**, Lecturer and Coordinator of Undergraduate Advising (919/515-7455); PhD, Chemical Engineering, Carnegie Mellon University (1991); multidisciplinary process design, teaching effectiveness, advising, educational outreach to K-12. [lisa\_bullard@ncsu.edu]

**Ruben G. Carbonell**, Frank Hawkins Kenan Distinguished Professor, Co-director of NSF Science and Technology Center for Environmentally Responsible Solvents and Processes, Director of the William R. Kenan Jr. Institute for Engineering, Technology and Science, and Director of the Kenan Center for Utilization of CO<sub>2</sub> in Manufacturing (919/515-5118); PhD, Chemical Engineering, Princeton University (1973); biochemical engineering, molecular recognition, bioseparations, immunodiagnostics, colloid and interface science, transport phenomena. [ruben@ncsu.edu]

**Joseph M. DeSimone**, Co-director of NSF Science and Technology Center for Environmentally Responsible Solvents and Processes and William R. Kenan, Jr. Professor (joint with Department of Chemistry, UNC-Chapel Hill) (919/962-2166); PhD, Polymer Chemistry, Virginia Tech (1990); polymer chemistry and physics, chemistry in compressed media, design of interfacially active agents for near and supercritical fluids, environmentally benign solvents for industrial processes. [desimone@unc.edu]

**Peter S. Fedkiw**, Associate Department Head and Professor (919/515-3572); PhD, Chemical Engineering, University of California, Berkeley (1978); electrochemical reaction engineering; electrocatalysis, environmental applications of electrochemistry. [fedkiw@eos.ncsu.edu]

**Jan Genzer**, Associate Professor (919/515-2069); PhD, Materials Science and Engineering, University of Pennsylvania (1995); physics of thin polymer films, interfacial polymer science, morphology control of heterophase polymers, structure/formation of polymer-based nanocomposites. [jan\_genzer@unity.ncsu.edu]

**Christine S. Grant**, Associate Professor (919/515-2317); PhD, Chemical Engineering, Georgia Institute of Technology (1989); surface and interfacial science, mass transfer, environmental engineering, green chemistry. [grant@eos.ncsu.edu]

**Keith E. Gubbins**, H. Clark Professor (919/513-2262); PhD, Chemical Engineering, University of London (1962); molecular modeling of nanostructured materials, thermodynamics and rate processes in nanoporous and structured materials. [keg@ncsu.edu]

**Carol K. Hall**, Alcoa Professor (919/515-3571); PhD, Physics, SUNY Stony Brook (1973); molecular thermodynamics and computer simulation, equations of state, polymer modeling, bioseparations, protein folding. [hall@turbo.che.ncsu.edu]

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**Saad A. Khan**, Professor and Director of Graduate Program (919/515-4519); PhD, Chemical Engineering, MIT (1985); rheology and microstructure of complex materials - gels, suspensions, associative and biopolymers. [khan@eos.ncsu.edu]

**Peter K. Kilpatrick**, Professor and Head (919/515-7121); PhD, Chemical Engineering, University of Minnesota (1983); surfactant and interfacial science, fluid microstructure, colloidal aggregates, phase equilibria, biotechnology. [peter-k@eos.ncsu.edu]

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**P. K. Lim**, Professor (919/515-2328); PhD, Chemical Engineering, University of Illinois (1979); interfacial phenomena, homogeneous catalysis, free radical chemistry. [lim@eos.ncsu.edu]

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**Gregory N. Parsons**, Professor (919/515-7553); PhD, Physics, NC State University (1990); surface reactions

and chemical processes in electronic materials synthesis, bonding structure and electronic properties of inorganic semiconductors and insulators, physics of thin film devices. [parsons@ncsu.edu]

**Steven W. Peretti**, Associate Professor (919/515-6397); PhD, Chemical Engineering, California Institute of Technology (1986); metabolic characterization and manipulation. [peretti@eos.ncsu.edu]

**George W. Roberts**, Director of Graduate Recruiting, Professor (919/515-7328); ScD, Chemical Engineering, MIT (1965); chemical reaction engineering, applied catalysis, chemical reactor analysis and design, pollution prevention and control, alternate fuels. [groberts@eos.ncsu.edu]

**Richard J. Spontak**, Professor (joint with Materials Science and Engineering) (919/515-4200); PhD, Chemical Engineering, University of California at Berkeley (1988); polymer microscopy and scattering, morphology/property design and characterization of nano/microstructured polymers and polymer nanocomposites, polymer physics. [rich\_spontak@ncsu.edu]

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**Orlin Velev**, Assistant Professor (919/513-4318); PhD, Physical Chemistry, University of Sofia and Bulgarian Academy of Sciences (1996); colloid science and engineering, colloidal interactions, self-assembly and crystallization, nano- and microstructures with photonic, optical and electrical functionality, biosensors. [odvelev@unity.ncsu.edu]

**Anka Veleva**, Assistant Research Professor (919/515-7176); PhD, Physical Chemistry, Bulgarian Academy of Sciences (1993); biomaterials, tissue engineering of vascular grafts, design of biomimetic surfaces, cell-based bioassays, clinical diagnostics. [anveleva@unity.ncsu.edu]

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