

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** PECASE: Developing Novel Scaffolds for Biological Molecules by Solving the I-QSAR Problem Using the Signature Molecular Descriptor

**Activation Amount:** \$50,000.00

**Agency:** Sandia National Laboratories

**Personnel:**

PI - Donald Visco, Chemical Engineering

**Abstract:**

The signature molecular descriptor is a very powerful and robust way to encode the local environment of a particular atom in a molecule. Work in this area by this research team have demonstrated this feature in several refereed journal articles, conference presentations, and invited speaking engagements. Much of this project's recent work has been on exploring the use of the signature molecular descriptor to solve the inverse design problem. As this technique matures, certain algorithmic bottlenecks have become apparent as we fine-tune this methodology against a variety of different problems. Current work focuses on fleshing out these issues and addressing them via several concurrent studies. Additionally, we also plan to generate some of these solutions in the lab and test them in order to feedback "real" information to evaluate the effectiveness of the methodology. In addition to the use of the signature molecular descriptor in the solution of the inverse design problem, we plan to explore signature as a tool in similarity searching of large chemical databases. Gleaning activity and functionality relationships through alignment of amino acids in a protein sequence against certain known alignments is a workhorse tool of those in the wide field of bioinformatics. The chemical landscape is very ripe for a similar procedure owing to the recent generation of very large chemical databases, including PubChem. In this portion of the work, we plan to explore the use of signature as the encoding device for any chemicals in order to facilitate the similarity searching of large chemical databases. The ultimate goal would be to find substances which score high on alignment relative to known (re: database) substances in a particular areas (re: therapeutics) in order to widen the candidate pool of substances in this area.

# ***Grants Awarded Report***

**From:** 3/1/09 to 3/31/09

**Project Title:** CAT National Dissemination: Assessment and Improvement of Learning/DUE-CCLI-Phase 3 (Comprehensive)

**Activation Amount:** \$100,000.00

**Agency:** National Science Foundation

**Personnel:**

PI - Barry Stein, Counseling and Psychology

Support Personnel - Mark T. Tylka,

**Abstract:**

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** Ecological Assessment of Wetland Inventory at Fort Campbell, Kentucky

**Activation Amount:** \$99,000.00

**Agency:** U. S. Army Corps of Engineers (via DOD)

**Personnel:**

Co-PI - Thomas Roberts, Biology

PI - Kenneth Morgan, Biology

Support Personnel - Yvette Clark, Water Center

**Abstract:**

Through the Cooperative Ecosystems Studies Unit (CESU), Tennessee Tech will perform a unified ecological assessment inventory to identify the presence or absence of wetlands within +/- 83,000 acres of training lands within Fort Campbell. The proposed work will consist of pre-fieldwork study of existing information related to wetland resources, an intensive survey of specified areas for indicators using resources for determining wetland abundance, development and implementation of work plans for adequate documentation of selected sites and compilation of final project reports and permanent project records.

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** Tennessee Teaching Quality Initiative Database and Website

**Activation Amount:** \$15,000.00

**Agency:** Tennessee Board of Regents

**Personnel:**

PI - Kevin Liska, Business Media Center

**Abstract:**

The purpose of this project is to work on the Teaching Quality Initiative (TQI) databases and to provide website enhancements.

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** Studies of Fluctuation Processes in Nuclear Collisions

**Activation Amount:** \$37,000.00

**Agency:** U. S. Department of Energy

**Personnel:**

PI - Sakir Ayik, Physics

**Abstract:**

This project continues the investigations of spinodal instabilities in charge asymmetric nuclear systems in the framework of the stochastic one-body transport theory, which was previously proposed by the PI and has emerged as a promising microscopic approach for describing dynamics of density fluctuations in heavy-ion collisions.

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** Governor's School for Information Technology Leadership 2009

**Activation Amount:** \$121,000.00

**Agency:** Tennessee Department of Education

**Personnel:**

PI - Curtis Armstrong, Decision Sciences and Management

**Abstract:**

The Governor's School for Information Technology Leadership gives students the opportunity to develop their knowledge of information technology and business leadership by developing a business plan for an Information Technology based business. This will include developing a viable product or service, identifying the target market, designing a marketing plan, developing the needed technology to support the business, and determining the budget and needed capital for the business. The goals of the curriculum are: to excite high school students about the rapidly growing area of information technology-based business; to add to the students' technology skills and increase the students' awareness of the potential business value of technology; to retain the best and brightest Tennessee students in Tennessee universities; and to develop the future economic development in Tennessee. Formal courses, supervised individual group projects, and experiential learning techniques will comprise the program.

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** Development of a Li-ion Battery Tool for Predicting Life and Performance for Satellite Orbit Operation Scenarios

**Activation Amount:** \$30,000.00

**Agency:** Global Aerospace Corporation

**Personnel:**

PI - Venkat Subramanian, Chemical Engineering

**Abstract:**

In this overall program, the PI will assist Global Aerospace Corporation (GAC), its consultants, and future industrial partners, in developing a highly fidelity, computationally-efficient, first principles-based software model to predict the behavior of rechargeable lithium-ion batteries under a wide set of conditions including extended calendar life (for both shelf life and on-bus trickle-charge conditions), low temperature operation, and wide variations in power loads for satellite applications for a number of Earth orbits. The key to this effort is developing computationally-efficient, full-physics models of Li-ion battery performance that are applicable for 3 types of Earth orbits of interest. The orbits include Geosynchronous Earth Orbit (GEO), Medium Earth Orbit (MEO) and Highly Elliptical Orbit (HEO). Under these profiles, batteries are subjected to minimum cycling and lengthy periods of continuous low rate charge. The goal is to provide a tool for managers and operations personnel to project life and performance of Li-ion batteries in GEO, MEO and HEO orbits.

# *Grants Awarded Report*

**From:** 3/1/09 to 3/31/09

**Project Title:** Testing a Model to Increase Vegetable Intake and Reduce Obesity Indices in Rural Families through Hydroponic Gardening

**Activation Amount:** \$43,310.00

**Agency:** U. S. Department of Agriculture

**Personnel:**

Co-PI - Janice Branson, Agriculture

PI - Melinda Anderson, Human Ecology

Support Personnel - Ellen Wolfe, Office of Research and Graduate Studies

Support Personnel - Melinda Swafford, Human Ecology

Support Personnel - Michael Allen, Mathematics

**Abstract:**

Obesity is a serious medical crisis in the United States. Prevention of obesity in children and adults is a national priority of several federal initiatives including Healthy People 2010, and the Dietary Guidelines for Americans. Tennessee Technological University, in partnership with a rural Tennessee high school, proposes to test a strategy for increasing vegetable intake and reducing obesity measures in rural adolescents and their families through the use of hydroponic gardening in a vocational classroom. Specifically, the cost effectiveness of hydroponic gardening to produce enough vegetables to significantly increase vegetable intake will be studied. The impact of consuming hydroponically-grown vegetables on two obesity measures (Body Mass Index and blood pressure) will be determined. High school vocational students and their parents who participate in this study will complete food records and food surveys at regular intervals during the two year study, and be measured for Body Mass Index and blood pressure. High school vocational students will learn to maintain the hydroponic gardening systems at their school, and be involved in the harvesting and consumption of a variety of fresh vegetables.