

U.S. Department of Energy
Office of Science

Proposal#

88230

APPLICATION/PROPOSAL COVER SHEET

DATE: 06/11/2002

TO: SC-13 Division of Materials Sciences and Engineering
(ATTN: Varma, Matesh)

THE ATTACHED APPLICATION/PROPOSAL IS FOR YOUR REVIEW & APPROPRIATE ACTION

INST: KENTUCKY, UNIVERSITY OF

Lexington, KY

P.I.(s): Stencel, John M.

TYPE OF

REQUEST: Progress Report

DATE RECEIVED: 06/11/2002

NO. OF COPIES: 1

AWARD NO.: DE-FG02-00ER45832

TITLE: Kentucky DOE/EPSCOR Program

NOTICE NO.: N/A

RENEWAL DATE:

THIS APPLICATION/PROPOSAL HAS BEEN GIVEN A PRELIMINARY ADMINISTRATIVE
REVIEW BY THE GRANTS AND CONTRACTS DIVISION, SC-64.

- THIS APPLICATION/PROPOSAL WAS ALSO SUBMITTED TO: N/A

- OTHER COMMENTS

KY DOE/EPSCoR
University of Kentucky
Center for Applied Energy Research
2540 Research Park Drive
Lexington, KY 40511-8410
606-257-0207 FAX 606-257-0318



KENTUCKY
EPSCoR
PROGRAM

STATEWIDE EPSCoR PROGRAM
Kentucky Science and
Technology Council, Inc.
200 West Vine St., Suite 420
Lexington, KY 40507
606-255-3511 FAX 258-2986

June 11, 2002

Melanie Becker
US Department of Energy
SC-132
19901 Germantown Road
Germantown, MD 20874

Dear Ms. Becker:

I attach the Progress Report for the Kentucky DOE EPSCoR Program. Please contact me at (859) 257-0250, or fax (859) 257-0207, should you have any questions or comments about it. Thank you.

Sincerely,

John M. Stencil
Director, KY DOE EPSCoR

Cc: M. Varma
M. Ochsenbein

PROGRESS REPORT

for

Kentucky DOE EPSCoR Program

June 2002

John M. Stencel and Melissa P. Ochsenbein
Center for Applied Energy Research
University of Kentucky
2540 Research Park Drive
Lexington, KY 40511
(859) 257-0250, stencel@caer.uky.edu

ABSTRACT

The KY DOE EPSCoR Program supports two research clusters. The Materials Cluster uses unique equipment and computational methods that involve research expertise at the University of Kentucky and University of Louisville. This team determines the physical, chemical and mechanical properties of nanostructured materials and examines the dominant mechanisms involved in the formation of new self-assembled nanostructures. State-of-the-art parallel computational methods and algorithms are used to overcome current limitations of processing that otherwise are restricted to small system sizes and short times. The team also focuses on developing and applying advanced microtechnology fabrication techniques and the application of microelectromechanical systems (MEMS) for creating new materials, novel microdevices, and integrated microsensors.

The second research cluster concentrates on High Energy and Nuclear Physics. It connects research and educational activities at the University of Kentucky, Eastern Kentucky University and national DOE research laboratories. Its vision is to establish world-class research status dedicated to experimental and theoretical investigations in strong interaction physics. The research provides a forum, facilities, and support for scientists to interact and collaborate in subatomic physics research. The program enables increased student involvement in fundamental physics research through the establishment of graduate fellowships and collaborative work.

PROGRAM RESEARCH STATUS

In the MEMS research, alternative processing techniques were identified and characterized for the microfabrication of novel sensors and devices. Techniques including micro-milling and drilling, micro-embossing, micro-molding, electroplating, micro-stamping, micro-lamination, SAMs, and wafer-level bonding have been investigated and then experimentally performed. Specific sensors and devices that were designed and fabricated have significant industrial and DOE applications in advanced packaging, electronic controls and data processing platforms needed for "smart sensor"

operations. Because of the level of expertise within MEMS, a new collaborative research effort was initiated with scientists and engineers at ORNL.

The research in nanostructures is focusing on the structural, electronic, magnetic, mechanical, and transport properties of silicon-based and carbon-based materials as well as identifying growth mechanisms during the formation of self-assembled nanostructures. It employs state-of-the-art tight-binding molecular dynamics with a linear scaling algorithm. Specific structures that have been studied, with results submitted and/or published, includes silicon nanorods, carbon nanotubes, organic thin film growth when ethylene molecules are bombarded on a diamond surface, and the nanostructures of Ge/Si(100), Si/Si(111), Mn/Si(100), and Ti/Si(111). The results have promising implications for nanoscale electronics, optoelectronics and nanoscale magnetism. Results have been described in the submission of 12 manuscripts, of which seven have been accepted in journals like Physical Review Letters, Physical Review B and Physics Reports. Collaborations have also been initiated with researchers at ORNL, Stanford University and the University of Florida.

Activity in the experimental subatomic physics research has focused on interactions with and experimentation at the Thomas Jefferson National Accelerator Facility (TJNAF). Design, construction and use of the Moeller polarimeter for Hall A at TJNAF has resulted in numerous, successful experiments in which national and international collaborations have been fostered. The development and subsequent optimization of the polarized helium-3 target enabled four experiments to be completed. Finally, significant progress was accomplished in the application of the detector on the PrimEx HYCAL calorimeter and within the Hall B, pair production luminosity monitor.

The theoretical high energy physics research concentrates on large-scale computer simulations, effective theories to account for symmetry and particle contents, and solvable models for defining structure of quantum chromodynamics (QCD). It examines CP symmetry violation effects to distinguish interactions between matter and antimatter and to provide evidence of new physics clearly different than determined by standard model (SM) predictions. The CP violation can only occur if all three generations of quarks contribute to a process involving the weak interaction, such as decays of particles containing different flavors of quarks. This work is being accomplished in collaboration with experimentalists at Fermi laboratory. It also entails supersymmetric QCD and string theory.

SIGNIFICANT ACCOMPLISHMENTS

Significant accomplishments include:

- ☐ Dr. Shudin Liu at the University of Louisville has been presented with a \$5,000 award as the Ralph E. Powe Junior Faculty by Oak Ridge Associated Universities.
- ☐ Dr. Chakram Jayanthi was recognized as a University Scholar at the University of Louisville.
- ☐ Dr. Robert. Keynton was selected for Outstanding Young Scientist Award by the Houston Society of Engineering in Medicine and Biology.
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September 14, 2001

Dr. Matesh Varma
US Department of Energy
19901 Germantown Road
Germantown, MD 20874

Dear Mat:

As you know, one of the co-principal investigators (Dr. Craig Grimes) in the Materials Research Cluster headed by Dr. Craig Grimes of the Kentucky DOE EPSCoR Program has moved to another university outside of Kentucky. His departure has been a significant loss to the University of Kentucky. However, the Kentucky DOE EPSCoR Subcommittee has assessed how to carry forward with its aggressive stance on creating, supporting and sustaining materials research excellence in Kentucky. We have determined that further strengthening the materials research at the University of Louisville, in cooperation with the MRSEC research centered at the University of Kentucky, provides opportunities and potential achievements not available in our previous program.

Therefore, we recommend that work described in the attached proposal - Optoelectronic Devices from One-Dimensional Nanowires and Carbon Nanotube Cilia for Microfluidic and Sensor Applications - be substituted as the principle direction for the funding which was previously directed through Dr. Grimes' research group. Along with the proposal is an abbreviated resume of the new co-principal investigator, Dr. Bruce Alphenaar, a revised budget and a review of the work by Dr. H.T. Henderson from the University of Cincinnati and Dr. D. J Beebe from the University of Wisconsin. Upon your approval, we will re-budget to enable the researchers to begin their work.

Thank you. Please contact me if you have questions.

Sincerely,

John M. Stencel
Director, KY DOE EPSCoR

Cc: M. Ochsenbein

RESEARCH DESCRIPTION

Optoelectronic Devices from One-Dimensional Nanowires

Optoelectronic devices fabricated from one-dimensional nanowires should show enhanced characteristics compared with those fabricated from bulk materials, due to optical and electrical confinement. These characteristics can be exploited to create high speed optoelectronic switches for telecommunication applications, or coherent photon emitters for quantum computation. We have recently developed a unique low-temperature vapor-liquid-solid synthesis method to create one-dimensional semiconductor nanowires. Using a plasma enhanced CVD process in the presence of low melting point gallium droplets we have succeeded in producing highly uniform, single crystal Si, GaN, and C nanowires with diameters down to 10 nm. The nanowire diameter is determined by the vapor solubility in the liquid phase, and can be controlled independently from the liquid droplet diameter. We plan to use this technique to fabricate one and zero dimensional optoelectronic devices. Our growth mechanism is ideally suited to produce one-dimensional wires with sharp material interfaces since growth occurs at relatively low temperatures (400°C) keeping interdiffusion rates low. In addition, it should be possible to modulate the one-dimensional doping profile by varying the gas composition during the growth process. This will allow us to produce one-dimensional optically active wires with sharp p-n junction doping profiles, or zero-dimensional optical cavities with hetero-interface confinement within the one-dimensional wire. Metal contacts to the nanowires will be defined using standard electron beam lithography techniques recently established in our laboratory. The photoluminescence and electro-optical emission spectrum will be measured using a CCD detector with the device temperature varied between 10-300K in an optical flow cryostat. We plan to investigate the influence of confinement on the electrical and optical characteristics in the one-dimensional and zero-dimensional geometries, and to optimize the optical characteristics by controlling the growth and material parameters. DOE interest in nanoscale optoelectronic devices is demonstrated by work being pursued in this area by Paul Alvisatos at Lawrence Berkeley Laboratory and Jeff Brinker at Sandia National Laboratories.

Carbon Nanotube Cilia for Microfluidic and Sensor Applications

Although carbon nanotubes are only 2-20 nm in diameter and a few microns in length, they are also flexible, robust and have a relatively low resistivity. We plan to take advantage of these unique mechanical and electrical properties to create electromechanically controlled, artificial cilia that can be used to propel fluids or to locally sense nanometer scale particles. Figure 1 is a schematic drawing of the device structure. Carbon nanotubes will be grown vertically in patterned regions of a quartz substrate using methods developed by the University of Kentucky

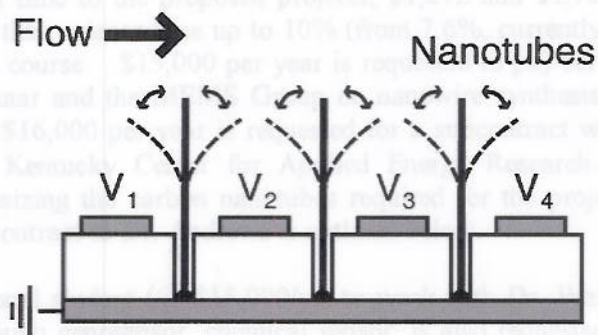


Figure 1. Schematic drawing of carbon nanotube cilia propelling a fluid using electrostatic deflection.

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- ☐ Dr. Kevin Walsh was presented with the University of Louisville Alumni Scholar for Research Award for outstanding research accomplishments.

- ☐ Theoretical calculations have successfully predicted the rate for black hole production by cosmic rays under low-scale gravity scenarios.
- ☐ The amount of extramural research funding awarded to Kentucky DOE EPSCoR Program researchers during the previous year was \$4,500,000.

PLANS & TIMETABLE FOR NEXT YEAR

The plans and timetable for the next year focus on increased interactions and experimentation with personnel at universities and the national laboratories, including Fermi, TJNAF, ORNL and Sandia. A high energy research conference is now scheduled at the University of Kentucky in Lexington, KY. Additional MEMS and nanoscale computational work is planned within the materials research cluster.

UNDERGRADUATES, GRADUATES AND POST DOCTORATES SUPPORTED BY THE DOE

The DOE funding supports three graduates, three undergraduates, and three postdoctorates. One minority student is supported by the DOE funds. These numbers represent less than 1/2 of the total number of students and post-doctorates participating in the KY DOE EPSCoR Program

KY DOE EPSCoR

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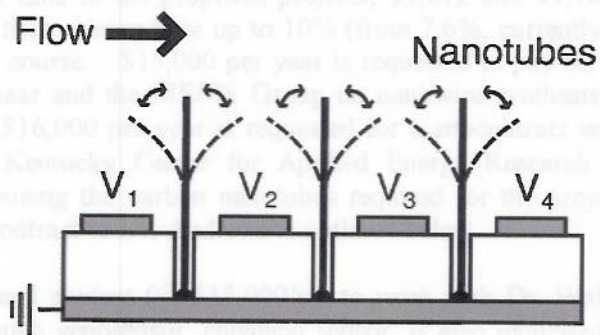


Figure 1. Schematic drawing of carbon nanotube cilia propelling a fluid using electrostatic deflection.

installation, maintenance and operation of the micromilling/drilling machine. In addition, \$20,000 is requested for the purchase of the micromilling/drilling machine due to the manufacturer making performance enhancement modifications on the system since the time of the original quote and to purchase a visualization system to magnify the field of view during the machining process. Finally, \$10,702 is requested for materials and supplies for nanodevice fabrication and low temperature measurements. Total annual cost including fringe benefits and overhead is \$94,867 from DOE and \$131,575 from the State (see attached budget forms for year 2, year 3 and summary).

**Project B: UofL - Walsh - Co-PI
2001-2002**

	DOE funds	State match	UofL match	Subtotals
A. Senior Personnel				
Dr. Bruce Alphenaar (UL EE)	4250	4250	0	8500
Dr. Kevin Walsh (UL EE)	936	936	0	1872
Dr. Rob Keynton (UL ME)	850	850	0	1700
Tommy Roussel	8106	6894	0	15000
Total Senior Personnel	14142	12930	0	27072
B. Other Personnel				
1 Post-doc	0	0	0	0
1 Microfab Technician	0	0	0	0
2 PhD Grad students	15000	15000	0	30000
Total Other Personnel	15000	15000	0	30000
Total Salaries (A+B)	29142	27930	0	57072
C. Fringe Benefits				
Faculty/Staff 24%	3394	3103	0	6497
Students 7.65% + \$756 Health Ins.	1904	1904	0	3807
Total Fringe	5298	5007	0	10304
TOTAL SALARIES, WAGES, FRINGES (A+B+C)	34440	32937	0	67376
D. Equipment				
Micro Milling/Drilling System	0	20000	0	20000
Inverted Microscope	0	0	0	0
Total Equipment (D)	0	20000	0	20000
E. Travel (domestic)	0	0	0	0
F. Participant Support Costs	0	0	0	0
G. Other Direct Costs				
Materials and Supplies	186	968	0	1154
Publication Costs	0	0	0	0
Other (see below)				
Subaward - UK - Dr. Andrews	0	16000	0	16000
UofL Tuition	0	0	15657	15657
Computer Services	0	0	0	
Consultant	0	0	0	
Total Other Direct Costs (G)	186	16968	15657	32811
H. Total Direct Costs (A thru G)	34626	69904	15657	120187
TDC less Equipment, Tuition & Subawards (base)	34626	33904	0	68530
I. Indirect Costs (44% of base)	15235	0	14918	30153
J. Total Direct and Indirect (H+I)	49861	69904	30575	150340

16903.5

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APPLICATION/PROPOSAL COVER SHEET

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- OTHER COMMENTS

Becker, Melanie

From: John Stencil [stencil@noah.caer.uky.edu]
Sent: Friday, May 25, 2001 2:44 PM
To: Becker, Melanie
Cc: melissa@caer.uky.edu; Matesh Varma
Subject: Kentucky DOE EPSCOR Progress Report



Progress Report May
2001.doc

Dear Melanie:

The Progress Report for Kentucky DOE EPSCoR is attached. Please contact me if questions should arise.

Sincerely,
John M. Stencil
Director, Kentucky DOE EPSCoR

PROGRESS REPORT

for

Kentucky DOE EPSCoR Program May 2001

John M. Stencil and Melissa P. Ochsenbein
Center for Applied Energy Research
University of Kentucky
2540 Research Park Drive
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(859) 257-0250, stencil@caer.uky.edu

ABSTRACT

The KY DOE EPSCoR Program supports two vibrant research clusters. The Materials Cluster builds upon the unique strengths and complementary expertise of researchers at the University of Kentucky and University of Louisville. Focused research in this team involves determining the physical, chemical and mechanical properties of nanostructured materials and isolating the dominant mechanisms involved in the formation of new self-assembled nanostructures. Another focus is on the development of advanced microtechnology fabrication techniques and the application of microelectromechanical systems (MEMS) for the development of new materials, novel microdevices, and integrated microsensors. State-of-the-art parallel computational methods and algorithms will be used to overcome current limitations of small system sizes and short times. This research is poised to place Kentucky at the forefront of microsensor and MEMS technology.

The second research cluster is in High Energy and Nuclear Physics. It connects research and educational activities at the University of Kentucky, Berea College, and Eastern Kentucky University. Its vision is to establish world-class research status dedicated to experimental and theoretical investigations in strong interaction physics. The research provides a forum, facilities, and support for scientists to interact and collaborate in subatomic physics research. Through the establishment of graduate fellowships and work with DOE national laboratories, the program enables increased student involvement in fundamental physics research.

PROGRAM RESEARCH STATUS

In the micro-sensor research, an array of magnetoelastic sensors has been fabricated for simultaneous measurement of temperature, pressure and humidity. The array is made of amorphous magnetoelastic, magnetostrictive materials that mechanically vibrate in response to time varying magnetic fields. The resonant frequency of the sensor depends on its elasticity and stress, in addition to its dimensions. The sensor tested had a cross-sectional dimension near 1mm.

The sensor fabricated also can be used to measure flow velocity, liquid density and liquid viscosity. Using other, specially developed polymers, the array can be used to measure CO₂, NH₃, pH and glucose concentrations. The range of values to be measured include: temperatures up to 350°C with precision 0.01°C; pressure up to 800PSI with precision 0.01PSI; fluid flow velocities up to 300 cm/s with precision 0.01cm/s; pH of 0.05 units; and CO₂ level differences of 1.0%.

The structure and stability of nanotori of different radii under mechanical deformation have been studied theoretically. The results are soon to appear in a manuscript submitted to Physical Review B. Using similar protocol, preliminary calculations on the structure, stability and mechanical properties of silicon nanorods have also been performed. These results show that the Young's modulus of a nanorod is different than the Young's modulus for bulk crystalline silicon. A paper is to be submitted to Physical Review B discussing reasons for the difference.

Other theoretical studies have determined that a very reliable Hamiltonian is needed if adsorption sites on Si surfaces are to be mapped. A tight-binding Hamiltonian, used for the work on Si nanorods, cannot be used for adsorption site work. Instead, the adsorption of either Si or Ge on a Si substrate has been shown to require a Hamiltonian with charge transfer and environment-dependent terms. Therefore, a new interaction Hamiltonian for Si and Ge is under development to help determine bonding and diffusion of adatoms on Si(111) and Si(100) surfaces.

The MEMS activity has focused on assembling a micro-capillary electrophoresis cell. This lab-on-a-chip design work has successfully constructed and tested the first prototype of a CEEC (capillary electrophoresis with electrochemical detection) device. It was decided that a small and reliable power supply would also be needed for the CEEC device. Therefore, a handheld battery-powered electronics package was constructed and successfully used to control the CEEC device.

Activity in the experimental subatomic physics research has focused on interactions with and experimentation at the Thomas Jefferson National Accelerator Facility (TJNAF). A test run was completed for the detector on the PrimEx HYCAL calorimeter. Simultaneously, construction was started on the Hall B, pair production luminosity monitor.

The theoretical high energy physics research concentrates on large-scale computer simulations, effective theories to account for symmetry and particle contents, and solvable models for defining structure of quantum chromodynamics (QCD). It examines CP symmetry violation effects to distinguish interactions between matter and antimatter and to provide evidence of new physics clearly different than determined by standard model (SM) predictions. The CP violation can only occur if all three generations of quarks contribute to a process involving the weak interaction, such as decays of particles containing different flavors of quarks. As a consequence, hyperon and B-meson decays are under investigation to examine if strong interaction effects contribute to CP violation in these decays. This work, accomplished in collaboration with experimentalists at Fermi laboratory, also entails supersymmetric QCD and string theory.

SIGNIFICANT ACCOMPLISHMENTS

Dr. 's Walsh and Keynton were awarded a NSF grant within the XYZ-on-a-Chip solicitation. It was one of 15 awards given by the NSF out of the 400 proposals that had been submitted.

Dr. Walsh was named the University of Louisville Alumni Scholar for Research for the period 1998-2000. This distinction, presented by the University, is given to a single faculty member of the Engineering School who best excels in the field of research.

PLANS & TIMETABLE FOR NEXT YEAR

The plans and timetable for the next year focus on increased interactions and experimentation with personnel at Fermi, TJNAF, ORNL and Sandia. A new faculty participant, with an emphasis on string theory, will join the high energy physics research team. Conferences are now being planned at the University of Kentucky for the summer 2002. Additional theoretical work is also planned in the nanotube research.

UNDERGRADUATES, GRADUATES AND POST DOCTORATES SUPPORTED BY THE DOE

The DOE funding supports 2.5 undergraduates, 2.5 graduates and 3.5 post-doctorates; this is $\frac{1}{2}$ of the total number of students and post-doctorates participating in the KY DOE EPSCoR Program.

Becker, Melanie

From: John Stencel [stencel@caer.uky.edu]
Sent: Thursday, May 12, 2005 11:27 AM
To: Becker, Melanie
Cc: Varma, Matesh
Subject: Continuation Progress Report for KY DOE EPSCoR



Progress Report,
04-05, to DOE...

Dear Melanie:

Attached is the Kentucky DOE EPSCoR Progress report. Please contact me if you have questions.

John Stencel
859-257-0250

Kentucky DOE EPSCoR Program

John M. Stencel and Melissa P. Ochsenbein, University of Kentucky, 2540 Research Park Drive, Lexington, KY 40511, tel (859) 257-0250; fax (859) 257-0302; stencel@caer.uky.edu

Introduction

The Kentucky DOE EPSCoR Program encompasses two cooperative Research Clusters at the University of Kentucky, University of Louisville and Northern Kentucky University. These research clusters have substantial interactions with DOE National Laboratories.

The Materials Research cluster focuses on theoretical and experimental investigations for understanding new nanoscale materials and MEMS techniques for creating novel microdevices and integrated microsensors. The theoretical studies examine the structural, electronic, magnetic and optical properties of single-walled carbon nanotubes, and Si and Si-Ge nanoclusters. The experimental MEMS research addresses advanced techniques for micro-milling/drilling, micro-embossing, micro-molding, electroplating, micro-stamping, micro-lamination, SAM's, wafer-level bonding, etchstop diffusion, and carbon nanotube growth.

The Theoretical Subatomic Physics Research Cluster focuses on understanding the nature of fundamental interactions of and between particles and fields. They include strong and weak interactions, as well as quantum gravity and other phenomena beyond the reach of existing experiments. The Cluster includes three research areas: phenomenological tests of the Standard Model (such as CP violation in heavy meson systems) which may point to new physics; theoretical extensions of the Standard Model, including supersymmetry and string theory; and tests extensions of these theories in areas such as predicting the presence and production of microscopic black holes in the earth's atmosphere.

Status

During the previous year in materials research advanced micro/nano-technology processing techniques were developed and used to fabricate novel micro-electromechanical system (MEMS) based sensors and devices. They were used to make microhotplates for gas sensing, microarrays for retinal stimulation, microtacks for tissue attachment, and carbon nanotube devices for MEMS and electronic applications. Custom electronic platforms were developed for wireless telemetric sensing. These achievements and the MEMS capabilities led to extensive collaborative research with personnel at ORNL, Sandia and Argonne.

Nanostructures of carbon, silicon, and self-assembled organic molecules were studied using theoretical calculations based on non-orthogonal tight-binding molecular dynamics and first principle molecular dynamics. Manuscripts were published detailing this innovative work and the research led to an invited review article in Physics Reports.

In high energy research, the theoretical explanation for and experimental evidence of microscopic black holes were investigated. Microscopic black holes could be regularly forming and exploding in the atmosphere above us. In theories of gravity that include several extra dimensions, the energies involved in cosmic ray collisions might be large enough to produce black holes. Such events could be observed in existing cosmic ray experiments. From the fact that cosmic ray showers of a predicted type have not yet been observed, we have obtained the best available limits on the size of extra dimensions. These limits will improve

over the next few years as additional data become available, and will be comparable to limits set by the Large Hadron Collider. On the other hand, if black hole cosmic rays are observed, they could provide the first evidence for extra dimensions, quantum gravity, and string theory.

Progress Status

The mission of the Kentucky DOE EPSCoR Program is to:

- foster sustainable improvements in research and human resources;
- establish national competitiveness in energy research of importance to Kentucky and the nation;
- support systemic change in science and engineering education;
- and, support training in enterprise development and entrepreneurship.

The research progress has been substantial and in-line with projected accomplishments during the previous year. smoothly. This progress is evidenced by the information presented in Table 1.

Table 1. Scientific manuscripts and presentations resulting from Kentucky DOE EPSCoR research during 2004.

Type	Manuscripts # Submitted	Manuscripts # Published	Presentations Type	Presentations #
Refereed Journal	36	29	Local	26
Non-Refereed	9	5	National	52
Book Chapter		2	International	15
Abstract		28		
Other		1		

Besides these scientific endeavors, KY DOE EPSCoR research has also provided innovations in technology development with the formation of two small companies attempting to commercialize their new products and the filing of the following US patents.

1. Z. Chen, Patent Application S.N. 60/388,638 (2002), Method to fabricate an ultra-short channel Si MOSFET using SWNT's as shadow masks.
2. R. Keynton, U.S. Provisional Patent Application Serial No. 10/364,658 (11/7/2003), A Capillary Electrophoresis-Electrochemical Microchip Device and Supporting Circuits.
3. K. Walsh, J. Lin, W. Hnat, M. Crain, J. Naber, D. Jackson, Patent Disclosure (9/24/03), MEMS-Based Capacitive Cantilever Train Sensor.
4. M. Crain, K. Walsh, T. Roussel, D. Jackson, R. Baldwin, R. Keynton, J. Naber, J. Edelen, US Patent Application (7/04), Microfab Capillary Electrophoresis with On-Chip Detection.
5. M. Martin, M. Crains, K. Walsh, Provisional Patent # P03019, University of Louisville (2/20/04), Lipid Bilayer Support Device, Lipid Regeneration Device and Systems.

Significant Findings

Recent discoveries within the Material Research Cluster at the University of Louisville have shed light on unusual electrical and magnetic properties of metallic carbon nanotori (Phys.

Rev. Lett. **88**, 217206, 2002). This work has prompted further studies on how to efficiently contact carbon nanotubes. Such an understanding is required for incorporating nanostructures into workable nanoscale devices, for example in ultra-sensitive magnetic sensors. Calculations on the electrical conductance of carbon nanotubes contacted by single-wall carbon nanotubes have provided the diagrams shown above. It is suggested that the differences between the right-contact and left-contact diminishes quantum interference of transmission as compared to the situation when the two contacts are equivalent.

In the High Energy Research Cluster at the University of Kentucky, microscopic black hole formation and explosion in our atmosphere are under investigation. In theories of gravity that include several extra dimensions, the energies involved in cosmic ray collisions might be large enough to produce these black holes. Such events could be observed in existing cosmic ray experiments. From the fact that cosmic ray showers of a predicted type have not yet been observed, we have obtained the best available limits on the size of extra dimensions. These limits will improve over the next few years as additional data become available, and will be comparable to limits set by the Large Hadron Collider. On the other hand, if black hole cosmic rays are observed, they could provide the first experimental evidence for extra dimensions, quantum gravity, and string theory.

Plans for the Next Year

The funding level from the DOE has decreased and will only be at \$155,000 during the next year. Hence, some research plans have been redirected because of the impact of funding. Nevertheless, the plans for the next year focus on continued interactions with and experimentation at Fermi, Sandia, TJNAF, ORNL and Argonne National Laboratories. The primary goal of the theoretical cluster's research program remains to gain insight into the nature of the fundamental interactions of particles and fields. These include the strong and weak interactions, as well as quantum gravity and other phenomena beyond the reach of existing experiments. In materials research, the structural, electronic, magnetic, mechanical, and transport properties of silicon-based and carbon-based nanostructures are to be elucidated further. The MEMS focus will continue with the development of new techniques and structures.

Students and Postdoctorates Supported

Table 2. Students, staff and postdoctorates supported by KY DOE EPSCoR.

	Females				Males				Total
	Asian American	Hispanic or Latino	White	Other	Asian American	Hispanic or Latino	White	Other	
Undergraduate	1		1				2		4
Grad. Students		1		4	1	2	2	3	13
Staff/Postdoc			1	1	2		6	3	13

Becker, Melanie

From: Varma, Matesh
Sent: Friday, March 19, 2004 8:29 AM
To: Becker, Melanie
Cc: Varma, Matesh
Subject: FW: Kentucky DOE EPSCoR Summary



Kentucky DOE
EPSCoR Program, s..
Mel:

Attached is the progress report from Kentucky John Stencel. Note change in budget and budget period.

FY 2003:	\$955,000	(KC020501)	07/01/03 - 10/31/04
		\$20,000	(KA140101)
		\$25,000	(KC020301)
FY 2004:	\$20,000	(KA140101)	07/01/04 - 08/31/05
	\$25,000	(KC020301)	
FY 2005:	\$110,000	(KC020501)	09/01/05 - 06/30/06
	\$20,000	(KA140101)	
	\$25,000	(KC020301)	
Total:	\$1,200,000		

Thanks.

Mat

-----Original Message-----

From: John Stencel [mailto:stencel@caer.uky.edu]
Sent: Thursday, March 18, 2004 6:30 PM
To: Varma, Matesh
Cc: Melissa Ochsenbein
Subject: Kentucky DOE EPSCoR Summary

Mat:
I attach a summary of our program. Please contact me if you have questions. John Stencel
(859) 257-0250

Kentucky DOE EPSCoR Program

March 19, 2004

John M. Stencel and Melissa P. Ochsenbein, University of Kentucky, 2540 Research Park Drive, Lexington, KY 40511, tel (859) 257-0250; fax (859) 257-0302; stencel@caer.uky.edu

Program Summary

The Kentucky DOE EPSCoR Program consists of two Research Clusters involving cooperative efforts between the University of Kentucky, University of Louisville, Northern Kentucky University and DOE National Laboratories.

The Materials Research cluster focuses on theoretical and experimental investigations for understanding new nanoscale materials and MEMS techniques for creating novel microdevices and integrated microsensors. The theoretical studies examine the structural, electronic, magnetic and optical properties of single-walled carbon nanotubes, and Si and Si-Ge nanoclusters. The experimental MEMS research addresses advanced techniques for micro-milling/drilling, micro-embossing, micro-molding, electroplating, micro-stamping, micro-lamination, SAM's, wafer-level bonding, etchstop diffusion, and carbon nanotube growth.

The Theoretical Subatomic Physics Research Cluster goal is to gain insight into the nature of the fundamental interactions of particles and fields. They include strong and weak interactions, as well as quantum gravity and other phenomena beyond the reach of existing experiments. The research focuses on three areas: phenomenological tests of the Standard Model (such as CP violation in heavy meson systems) which may point to new physics; theoretical extensions of the Standard Model, including supersymmetry and string theory; and tests of these extensions (such as predictions about the production of microscopic black holes).

Program Accomplishments

The Materials Research cluster has published more than 30 refereed manuscripts in journals such as Science, Physical Review Letters, Applied Physics Letters and Journal of Micromechanics and Microengineering. Research findings were highlighted in contributed and plenary presentations at national and international scientific and engineering conferences, and six US patents applications were filed. The results were also summarized for general audiences in web-based, magazine and journal venues, including PhysicsWeb, BBC News Online Health, the South African radio program "Future Watch," and 8 trade magazines such as Biophotonics International, Clinica, Medical Tribune, RAD, RT Image, Small Times, Surgical Rounds, and The Engineer. Non-EPSCoR funding was obtained from NSF, NASA, NRL and NIH.

The Theoretical Subatomic Physics Research Cluster published 10 refereed manuscripts and presented 4 papers at national and international scientific conferences. The work has garnered over 300 scientific citations (according to SPIRES database), and was featured in Physical Review Focus and Nature. The results were also summarized for general audiences in journalistic venues, including Science News and USA Today. Non-EPSCoR proposals were funded by the NSF and DOE.

Face Page

TITLE OF PROPOSED RESEARCH: Kentucky DOE EPSCoR Program

1. CATALOG OF FEDERAL DOMESTIC ASSISTANCE #:

81.049

2. CONGRESSIONAL DISTRICT:

Applicant Organization's District: 6th

Project Site's District: 6th, 3rd

3. I.R.S. ENTITY IDENTIFICATION OR SSN:

61-6033693

4. AREA OF RESEARCH OR ANNOUNCEMENT TITLE/#:

DOE EPSCoR Renewal Application

5. HAS THIS RESEARCH PROPOSAL BEEN SUBMITTED
TO ANY OTHER FEDERAL AGENCY?

Yes No X

PLEASE LIST:

6. DOE/OER PROGRAM STAFF CONTACT (if known):

Dr. Matesh Varma

7. TYPE OF APPLICATION:

New Renewal X
Continuation X Revision
Supplement

15. PRINCIPAL INVESTIGATOR/PROGRAM DIRECTOR
NAME, TITLE, ADDRESS, AND PHONE NUMBER

Dr. John M. Stencel
Center for Applied Energy Research
University of Kentucky
2540 Research Park Drive
Lexington, KY 40511
(859) 257-0250

OFFICIAL FILE COPY

SIGNATURE OF PRINCIPAL INVESTIGATOR/
PROGRAM DIRECTOR

John M. Stencel
12/16/02
Date

PI/PD ASSURANCE: I agree to accept responsibility for the scientific conduct of the project and to provide the required progress reports if an award is made as a result of this submission. Willful provision of false information is a criminal offense. (U.S. Code, Title 18, Section 1001).

NOTICE FOR HANDLING PROPOSALS

This submission is to be used only for DOE evaluation purposes and this notice shall be affixed to any reproduction or abstract thereof. All Government and non-Government personnel handling this exercise extreme care to ensure that the information contained herein is not duplicated, used, or disclosed in whole or in part for any purpose other than evaluation without written permission. If an award is made based on this submission, the terms of the award shall control disclosure and use. This notice does not limit the Government's right to use information contained in the submission if from another source without restriction. This is a Government notice, and shall not itself be construed to impose any liability upon the Government or Government personnel for any disclosure or use contained in this submission.

PRIVACY ACT STATEMENT

If applicable, you are requested, in accordance with 5 U.S.C., Sec. 552A, to voluntarily provide your Social Security Number (SSN). However, you will not be denied any right, benefit, or privilege provided law because of a refusal to disclose your SSN. We request your SSN to aid in accurate identification, referral and review of applications for research/training support for efficient management of Off grant/contract programs.

8. ORGANIZATION TYPE:

Local Govt.	<u> </u>	State Govt.	<u> </u>
Non-Profit	<u> </u>	Hospital	<u> </u>
Indian Tribal Govt.	<u> </u>	Individual	<u> </u>
Other	<u> </u>	Inst. of Higher Edu	<u>X</u>
For-Profit	<u> </u>		
Small Business	<u> </u>	Disadvan. Business	<u> </u>
Women-Owned	<u> </u>	8(a)	<u> </u>

9. CURRENT DOE AWARD # (IF APPLICABLE):

DE-FG02-00ER45832

10. WILL THIS RESEARCH INVOLVE:

10A Human Subjects No X If yes,
Exemption No. or
IRB Approval Date
Assurance of Compliance No:
10B Vertebrate Animals No If yes,
IACUC Approval Date
Animal Welfare Assurance No:

11. AMOUNT REQUESTED FROM DOE FOR ENTIRE

PROJECT PERIOD \$ 2,250,000

12. DURATION OF ENTIRE PROJECT PERIOD:

7/1/2003 to 6/30/2006
Mo/day/yr. Mo/day/yr.

13. REQUESTED AWARD START DATE

7/1/2003 (Mo/day/yr.)

14. IS APPLICANT DELINQUENT ON ANY FEDERAL DEBT?

Yes (attach an explanation) No X

16. ORGANIZATION'S NAME, ADDRESS AND CERTIFYING
REPRESENTATIVE'S NAME, TITLE, AND PHONE NUMBER

Jack Supplee
Associate Director, UKRF
University of Kentucky
102 Kinkead Hall
Lexington, KY 40506
(859) 257-9420

SIGNATURE OF ORGANIZATION'S CERTIFYING
REPRESENTATIVE

Jack Supplee
12-17-02
Date

CERTIFICATION & ACCEPTANCE: I certify that the statements herein are true and complete to the best of my knowledge, and accept the obligation to comply with DOE terms and conditions of this submission. A willfully false certification is a criminal offense. (U.S. Code, Title 18, Section 1001).

U.S. Department of Energy
YEAR 1 BUDGET for KY DOE EPSCoR Program
 (See reverse for instructions)

ORGANIZATION University of Kentucky Research Foundation				Budget Page No. <u>1</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Dr. John M. Stencel				Req Duration: <u>12</u> (Months) 7/01/03 - 6/30/04		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty, & Senior Associates <small>(List each separately with title, A-7, show number in brackets(s))</small>				DOE Funds Requested by Applicant	State Match	University Match
	CAL	ACAD	SUMR			
1. J. M. Stencel	6			\$30,387	\$0	\$21,705
2. M. P. Ochsenbein	6			\$21,547	\$0	\$0
3. C. S. Jayanthi			1	\$4,707	\$4,707	\$0
4. K. Walsh	2			\$0	\$18,000	\$0
5. A. D. Shapere		4.05		\$0	\$5,949	\$20,822
6. (12) OTHERS (LIST INDIVIDUALLY ON BUDGET EXPLANATION)	51	4.95	3	\$110,866	\$118,483	\$33,431
7. (17) TOTAL SENIOR PERSONNEL (1-6)	65	9	4	\$167,507	\$147,139	\$75,958
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (4) POST DOCTORAL ASSOCIATES	12	36	0	\$86,000	\$70,000	\$0
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER,	3			\$0	\$8,342	\$0
3. (11) GRADUATE STUDENTS				\$36,626	\$156,626	\$0
4. (2) UNDERGRADUATE STUDENTS				\$4,667	\$2,333	\$0
5. () SECRETARIAL-CLERICAL				\$0	\$0	\$0
6. () OTHER				\$0	\$0	\$0
TOTAL SALARIES AND WAGES (A+B)				\$294,800	\$384,440	\$75,958
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$58,790	\$68,925	\$2,442
TOTAL SALARIES, WAGES, AND FRINGE BENEFITS (A+B+C)				\$353,590	\$453,365	\$78,400
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)						
IBM P-Series, e-beam evaporator						
Computer Workstations (2), Color Printer						
TOTAL PERMANENT EQUIPMENT				\$176,685	\$12,430	\$0
E. TRAVEL						
1. DOMESTIC (incl. Canada & U.S. Possessions)				\$21,550	\$10,515	\$0
2. FOREIGN				\$8,350	\$6,500	\$0
TOTAL TRAVEL				\$29,900	\$17,015	\$0
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$0	\$0	\$0
2. TUITION AND FEES				\$0	\$0	\$0
3. TRAINEE TRAVEL				\$0	\$0	\$0
4. OTHER (fully explain on justification page)				\$0	\$0	\$0
TOTAL PARTICIPANTS () TOTAL COST				\$0	\$0	\$0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES				\$8,987	\$44,042	\$0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$1,500	\$2,000	\$0
3. CONSULTANT SERVICES				\$5,458	\$11,196	\$0
4. COMPUTER (ADP) SERVICES				\$0	\$0	\$0
5. SUBCONTRACTS (UK, NKU, Louisville Science Center)				\$43,038	\$37,702	\$1,550
6. OTHER (Graduate Student Tuition)				\$18,400	\$22,250	\$43,678
TOTAL OTHER DIRECT COSTS				\$77,383	\$117,190	\$45,228
H. TOTAL DIRECT COSTS (A THROUGH G)				\$637,558	\$600,000	\$123,628
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS				\$112,442	\$0	\$391,498
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$750,000	\$600,000	\$515,126
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$1,115,126		
L. TOTAL COST OF PROJECT (J+K)				\$1,865,126		

U.S. Department of Energy
YEAR 2 BUDGET for KY DOE EPSCoR Program
 (See reverse for instructions)

ORGANIZATION University of Kentucky Research Foundation				Budget Page No. 2		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Dr. John M. Stencel				Req Duration: 12 (Months) 7/01/04 - 6/30/05		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty, & Senior Associates (List each separately with title. A.7. show number in brackets(s))				DOE Funds Requested by Applicant	State Match	University Match
	CAL	ACAD	SUMR			
1. J. M. Stencel	6			\$27,088	\$0	\$27,088
2. M. P. Ochsenbein	6			\$22,409	\$0	\$0
3. C. S. Jayanthi			1	\$4,989	\$4,707	\$0
4. K. Walsh	2			\$0	\$18,000	\$0
5. A. D. Shapere		3.6		\$0	\$3,094	\$21,655
6. (12) OTHERS (LIST INDIVIDUALLY ON BUDGET)	51	4.5	3	\$112,974	\$114,635	\$34,768
7. (17) TOTAL SENIOR PERSONNEL (1-6)	65	8.1	4	\$167,460	\$140,436	\$83,511
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (4) POST DOCTORAL ASSOCIATES	12	36		\$90,400	\$70,000	\$0
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PR)	2			\$0	\$5,784	\$0
3. (11) GRADUATE STUDENTS				\$38,991	\$158,091	\$0
4. (2) UNDERGRADUATE STUDENTS				\$4,853	\$2,427	\$0
5. () SECRETARIAL/CLERICAL				\$0	\$0	\$0
6. () OTHER				\$0	\$0	\$0
TOTAL SALARIES AND WAGES (A+B)				\$301,704	\$376,738	\$83,511
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$64,638	\$68,329	\$5,756
TOTAL SALARIES, WAGES, AND FRINGE BENEFITS (A+B+C)				\$366,342	\$445,067	\$89,267
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)						
IBM P-Series 670, Spectrometer and CCD Detector						
Upgrade to Sputter System, CV System						
Computer Workstation (1)						
TOTAL PERMANENT EQUIPMENT				\$171,747	\$5,697	\$0
E. TRAVEL						
1. DOMESTIC (incl. Canada & U.S. Possessions)				\$23,400	\$12,615	\$0
2. FOREIGN				\$1,500	\$14,025	\$0
TOTAL TRAVEL				\$24,900	\$26,640	\$0
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$0	\$0	\$0
2. TUITION AND FEES				\$0	\$0	\$0
3. TRAINEE TRAVEL				\$0	\$0	\$0
4. OTHER (fully explain on justification page)				\$0	\$0	\$0
TOTAL PARTICIPANTS () TOTAL COST				\$0	\$0	\$0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES				\$9,781	\$45,402	\$0
2. PUBLICATION COSTS/DOCUMENTATION/DISEMINATION				\$1,500	\$2,000	\$0
3. CONSULTANT SERVICES				\$4,603	\$14,808	\$0
4. COMPUTER (ADP) SERVICES				\$0	\$0	\$0
5. SUBCONTRACTS (UK, NKU, Louisville Science Center)				\$43,714	\$38,136	\$1,679
6. OTHER (Graduate Students Tuition)				\$20,400	\$22,250	\$44,178
TOTAL OTHER DIRECT COSTS				\$79,998	\$122,596	\$45,857
H. TOTAL DIRECT COSTS (A THROUGH G)				\$642,987	\$600,000	\$135,124
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS				\$107,013	\$0	\$390,799
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$750,000	\$600,000	\$525,923
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$1,125,923		
L. TOTAL COST OF PROJECT (J+K)				\$1,875,923		

U.S. Department of Energy
YEAR 3 BUDGET for KY DOE EPSCoR Program
 (See reverse for instructions)

ORGANIZATION University of Kentucky Research Foundation				Budget Page No. <u>3</u>		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Dr. John M. Stencel				Req Duration: <u>12</u> (Months) 7/01/05 - 6/30/06		
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty, & Senior Associates <small>(List each separately with title, A.T. show number in brackets(s))</small>				DOE Funds Requested by Applicant	State Match	University Match
	CAL	ACAD	SUMR			
1. J. M. Stencel	6			\$32,867	\$0	\$23,476
2. M. P. Ochsenbein	6			\$23,305	\$0	\$0
3. C. S. Jayanthi			1	\$5,238	\$4,707	\$0
4. K. Walsh	2			\$0	\$18,000	\$0
5. A. D. Shapere		3.6		\$0	\$3,217	\$22,521
6. (12) OTHERS (LIST INDIVIDUALLY ON BUDGET EX	51	4.5	3	\$115,141	\$114,801	\$36,159
7. (17) TOTAL SENIOR PERSONNEL (1-6)	65	8.1	4	\$176,551	\$140,725	\$82,156
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. (4) POST DOCTORAL ASSOCIATES	12	36		\$94,967	\$45,722	\$0
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRA	3			\$0	\$9,023	\$0
3. (11) GRADUATE STUDENTS				\$41,442	\$159,615	\$0
4. (2) UNDERGRADUATE STUDENTS				\$5,047	\$2,524	\$0
5. () SECRETARIAL-CLERICAL				\$0	\$0	\$0
6. () OTHER				\$0	\$0	\$0
TOTAL SALARIES AND WAGES (A+B)				\$318,007	\$357,609	\$82,156
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				\$59,061	\$68,497	\$2,641
TOTAL SALARIES, WAGES, AND FRINGE BENEFITS (A+B+C)				\$377,068	\$426,106	\$84,797
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM) IBM P-Series 670, upgrade to sputter system, CV System						
TOTAL PERMANENT EQUIPMENT				\$162,709	\$3,471	\$0
E. TRAVEL						
1. DOMESTIC (incl. Canada & U.S. Possessions)				\$13,894	\$21,441	\$0
2. FOREIGN				\$0	\$14,576	\$0
TOTAL TRAVEL				\$13,894	\$36,017	\$0
F. TRAINEE/PARTICIPANT COSTS						
1. STIPENDS (itemize levels, types + totals on budget justification page)				\$0	\$0	\$0
2. TUITION AND FEES				\$0	\$0	\$0
3. TRAINEE TRAVEL				\$0	\$0	\$0
4. OTHER (fully explain on justification page)				\$0	\$0	\$0
TOTAL PARTICIPANTS () TOTAL COST				\$0	\$0	\$0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES				\$9,576	\$44,855	\$0
2. PUBLICATION COSTS/DOCUMENTATION/DISEMINATION				\$1,500	\$2,000	\$0
3. CONSULTANT SERVICES				\$8,709	\$26,732	\$0
4. COMPUTER (ADP) SERVICES				\$0	\$0	\$0
5. SUBCONTRACTS (UK, NKU, Louisville Science Center)				\$44,355	\$38,569	\$1,809
6. OTHER (Tuition)				\$22,400	\$22,250	\$44,694
TOTAL OTHER DIRECT COSTS				\$86,540	\$134,406	\$46,503
H. TOTAL DIRECT COSTS (A THROUGH G)				\$640,211	\$600,000	\$131,300
I. INDIRECT COSTS (SPECIFY RATE AND BASE)						
TOTAL INDIRECT COSTS				\$109,789	\$0	\$405,020
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$750,000	\$600,000	\$536,320
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$1,136,320		
L. TOTAL COST OF PROJECT (J+K)				\$1,886,320		

A-4

BUDGET JUSTIFICATION FOCUS GROUP "A"

SALARY COSTS

- A. Salaries for senior personnel have been requested at the following levels: 1-month summer salaries for Dr. Jayanthi, Dr. Sumanasekea, and Dr. Wu with 3% annual increase and 12-month calendar year salaries for two research assistant professors (Dr. Liu and Dr. Yu) with ~2% annual increase. Dr. Liu will work on projects devoted to carbon nanotubes, while Dr. Yu will work on projects related to silicon nanostructures.

- B. One postdoctoral associate @ \$32,000/yr has been requested from the Kentucky state portion of the budget. This postdoc will primarily work on the project on DWCNT-based metal-semiconductor junction. Two graduate research assistants will also be involved in this proposal. One GRA will work on the synthesis and characterization of quasi-one-dimensional nanostructures and the other one will be involved in the modeling of nanoscale devices. The total salary costs for the two GRA's are \$30,000 (yr.1), \$30,900 (yr.2), and \$31,827 (yr.3). Annual salary increments of 3% are requested for GRAs and postdocs and they are charged to the DOE portion of the budget.

C. FRINGE BENEFITS

Fringe benefits have been calculated at 24% for the faculty, 17% for the post-doctoral associate, and 7.65% for graduate students. Health insurance coverages for the two GRAs have been requested. They are charged to the state funds at the following rates per student: \$935 (yr. 1), \$ 963 (yr. 2), and \$991 (yr. 3).

D. EQUIPMENT

Funds have been requested to purchase a IBM p-series 670 Unix server (Model 7040-671) that has the following specifications: 16-way SMP with power4 processor, 16 GB memory, 1.1 GHz, 70 Gflops , 288 GB disk drive, and 160 GB tape drive. This Unix server will be dedicated to the proposed projects on large-scale molecular dynamics simulations of nanoscale structures and devices. The University of Louisville price of this computer is \$240,000. IBM has agreed to accept payments on this computer in three installments (Year 1: \$96,801, Year 2: \$54,163, and Year 3: \$88,934). For the experimental component of this project, a spectrometer has been requested for Raman characterization of nanostructures. The spectrometer is a Triax 550 Monochromator with a front-illuminated CCD detector (204bx512 pixels). The quoted price of the spectrometer+CCD detector is \$39,902.

E. TRAVEL (~\$9660/yr)

Travel funds have been requested to attend the DOE-sponsored workshops on nanophase materials and to present talks at national conferences (e.g. APS, MRS, etc.) by the participants of this project. Travel funds have been set-aside for visits related to research collaborations: (i) 3-visits/yr to Pennsylvania State University (Dr. Eklund's group) by either Dr. Sumanasekera or his students to perform micro-Raman measurements, (ii) 2-visits/yr to ORNL to collaborate with the members of the theory group of the center for nanophase materials, (iii) Dr. Wu's visit to LLNL, (iv) Dr. Jayanthi's visit to the University of Nijmegen, Institute of Theoretical Physics, The Netherlands (Prof. Fasolino's group), and (v) Prof. Wu's visit to National Taiwan University (Prof. Guo's group). Letters of intent to collaborate with these research groups are enclosed.

F. OTHER DIRECT COSTS

Materials and Supplies

Theory Group (~\$2000/yr): These funds have been requested for two refills of color toners (2x\$610=1220), two refills of black laser toners for the laser printer used by post-docs/students (\$130); CDs, tapes, and zip disks for data back-ups (\$200), and conference presentation materials such as posters and transparencies (\$400/yr with ~3 posters/yr and 2 boxes of transparencies). Typical costs for preparing a color poster is ~\$100/poster and for purchasing a box of 50 sheets of color transparencies is \$50.

Experimental Group (~\$4000/yr): 10 re-fills of Liquid Helium (30 liters at \$7/liter = \$2100), Liquid Nitrogen (\$700/yr), AFM tips (\$300/yr), raw materials (graphite and silicon powders), gases (Ar. He, He-

Materials Research

Hydrogen mixture, oxygen, propane) and catalysts (Co, Fe, Ni, etc) required in synthesis of carbon nanotubes and silicon-based nanostructures (\$900/yr).

Publication Costs (\$2500/yr) The amount requested is to defray publication charges (~ 12 pages/year) and reproduction costs associated with color figures.

Consultant (\$2500/yr) A Sacred Heart high-school teacher (Ms. Nancy P. Miller) will be hired as a consultant to coordinate the educational activities outlined in this proposal. She will be the liaison between our research group, the Louisville Science Center, and the high-school students from the Louisville Metropolitan area. The consultant costs are charged to the state funds.

Others

- Hardware Maintenance charges of the Unix Server: \$ 17,000/yr
- License renewals and updates of software packages (VASP, DMOL, IMSL, NAG, etc) - \$3000/yr
- A part-time computer system assistant will be used to operate the access-grid facility whenever seminars/colloquia on nanoscience/nanotechnology are broadcast over the network from participating universities and national laboratories, for web-designing tasks, and computer maintenance tasks (\$2500/yr).

Subawards

University of Kentucky (\$131,107) : A sub-award is provided to the University of Kentucky for the research work carried out by Dr. Zhi-Chen (Electrical Engineering) on device-related applications of double-wall carbon nanotubes. The sub-award requests funds for 1-month summer salary (8011/yr), a graduate student stipend (~\$14,400 /yr), tuition costs (\$4600 -yr1, \$5100-yr2, and 5600-yr3), fringe benefits (\$3872/yr), travel (\$1500/yr), and materials and supplies (~\$3000/yr). The indirect cost used by the sub-award is 47% in year 1 and 47.3% for subsequent years.

Louisville Science Center (\$2500/yr): A sub-award will be provided to Ms. Amy Lowen and Ms. Theresa Mattei of the Louisville Science Center (LSC) for the outreach and educational components of this proposal. This budget will be used to initiate, develop and implement the nanoscience and nanotechnology educational program at the Louisville Science Center. For example, the funds will be used to develop educational kits, to underwrite the staff time for the project-coordinator and to defray teleconferencing charges in broadcasting the nanoscience/nanotechnology program over the KTLN network to participating high schools in the commonwealth of Kentucky.

G. INDIRECT COSTS Indirect cost charged by the University of Louisville is 46% (Yr. 1) and 47% for subsequent years with the modified total direct cost computed using the formula (TDC- Equipment- excess of \$25,000 for *each* subcontract). No indirect has been charged to the state portion of the fund. The state portion of the indirect has been added to the indirect portion of the university contributions.

H. COST SHARING University of Louisville will provide tuition remission for two GRAs identified to work on this project.

I. TOTAL COST OF THE PROJECT

	<u>DOE</u>	<u>STATE</u>	<u>LOCAL</u>
Year 1	\$208,440	\$208,734	\$112,695
Year 2	\$204,418	\$208,868	\$115,346
Year 3	\$204,152	\$209,534	\$116,175
Cumulative	\$617,010	\$627,136	\$344,216

BUDGET JUSTIFICATION FOCUS GROUP "B"

The total cost of this three-year project is \$1,836,642 of which \$718,783 is from DOE, \$387,346 from the University of Louisville, and \$730,513 from the State of Kentucky.

The University of Louisville and the State of Kentucky recognize the importance and potential impact that this project will have on research and educational activities in the state and have elected to make a very strong financial commitment to ensure its success. The total cost share being provided for this project is over 60% of the total project costs. Details of the project costs and cost sharing appear below.

Senior Personnel. There are 8 senior investigators listed on the proposal. Each will be responsible for a specific, well-defined portion of the project. Dr. Kevin Walsh (ECE) has over 14 years of MEMS/uFab experience and will serve as the PI/PI for the overall Focus Area B project. He will also lead the team designing the MEMS-based micro-calorimeter in collaboration with ORNL. Dr. Robert Keynton (ME) is an expert in bio-MEMS, cardiovascular research, and alternative microfabrication techniques for MEMS. He will serve as project leader on the bio-electronic sensor project, as well as coordinator for investigations into alternative fabrication technologies. Dr. Bruce Alphenaar (ECE) is an expert in nanotechnology and molecular electronics. He will work with Dr. Bruce Hinds (UK - Chem and Materials Eng) on the nanotechnology molecular electronics project. Dr. Rick Baldwin (Chemistry) is an expert in analytical electrochemistry and will serve as project leader for the lab-on-a-chip (LOC) project. Dr. John Naber (ECE) is an expert in the fields of custom electronics and wireless communications. He will head the team performing research for the wireless retinal implant prosthetic device. Mark Crain is a senior engineer and cleanroom operations manager with a background in ME, EE, MEMS and microfabrication. He will coordinate all microfabrication activities both inside and outside the cleanroom and aid in the design of the custom MEMS devices. The final person listed is a senior research scientist (Mike Martin) who will be responsible for the following: nanotechnology fabrication, carbon nanotube growth, and LOC fabrication and testing. Teaching release time is requested for Drs. Walsh, Keynton, Alphenaar, Naber and Baldwin. Teaching release for Dr. Hinds of UK appears in the subcontract listed below. In summary, Senior Personnel Costs total \$429,000 (\$270,000 from DOE and \$159,000 from KY).

Other Personnel. Other personnel support in this 3-year effort includes 5 full-time Graduate Students, one each dedicated to the 5 different projects. Yearly stipends for these positions are \$18K/yr/student. Other Personnel Costs total \$270,000 (\$270,000 from KY).

Fringe Benefits. A fringe benefit rate of 24% is used for the faculty and research scientists/engineering positions. Fringe on the graduate student positions is 7.65%. Health Insurance for the graduate students is \$1000/yr/student. Fringe Costs total \$138,615 (\$64,800 from DOE and \$73,815 from KY).

Equipment. \$236,441 is required for capital equipment for the following critical items: a multi-pocket, multi-gun e-beam evaporator with heated substrate control and film thickness monitor for deposition of the thin films required by the MEMS devices and molecular electronics (\$150,000), an upgrade to our existing sputtering system to include mass flow controllers and PC control (\$60,000), and an CV system for determining doping profiles (\$26,441). (\$227,743 from DOE and \$8,698 from KY)

Travel. \$15,000 over the three years will be used for travel to domestic conferences and national laboratories to present results and discuss technical issues with our DOE collaborators. The total will cover all travel expenses (meals, air, lodging) for an average of one overnight trip for 6 members of the group per year. Refer to the budget sheet for a breakdown of these expenses. (\$15,000 from KY)

Other Direct Costs. \$285,000 of Other Direct Costs is requested for this project (\$204,000 from KY and \$81,000 from UL). Other Direct Costs includes Cleanroom Equipment usage at the traditional rate of \$1,000/month/person (\$10,000/yr), other Materials and Supplies not related to Cleanroom Equipment usage such as biological needs, custom MEMS needs, electronics, and packaging (\$24,000/yr), MEMCAD modeling software (\$3,000/yr), publication costs (\$1,000/yr), subcontract to UK for Dr. Hinds' research (\$90,000) and Tuition for the 5 UofL graduate students over 3 years (\$81,000).

Indirect Costs. A 46% indirect cost rate is applied to the Project Total Direct Costs less the costs associated with Capital Equipment and Tuition for the first year, and 47% thereafter.

Matching or Cost Share. The University is providing \$387,346 of cost share as support of this critical research project. The State of Kentucky is providing an additional \$730,513 of cost share funding. The total cost share amount equals 60% of the requested Federal funding.

TOTAL COST OF THE FOCUS GROUP "B" PROJECTS

	<u>DOE</u>	<u>STATE</u>	<u>LOCAL</u>
Year 1	\$242,820	\$243,135	135,378
Year 2	\$238,136	\$243,302	125,984
Year 3	\$237,827	\$244,076	125,984
Cumulative	\$718,783	\$730,613	387,346

Budget Explanation

The total budget request to the DOE for this proposal is \$600,168 for the three year period; \$199,860 for the first year, \$200,290 for the second year and \$200,018 for the third year. The requested budget from the State of Kentucky is \$394,169 total; \$130,928 in Year 1, \$133,161 in Year 2, and \$130,079 in Year 3.

The co-PIs will be supported by the University of Kentucky's salary matching contribution. 30% of Das and Shapere's academic year salaries and 10% of Gardner's salary will be contributed to the project. The grant will contribute 10% of Das and Shapere's academic year salaries in Year 1 and 5% in Years 2 and 3 towards outreach activities, which will be matched by a 5% contribution from the University. Das and Shapere each expect to spend an average of 6 hours per week of the academic year on these outreach activities in Year 1, and 4 hours per week in subsequent years. Prof. Das's outreach time in Year 1 will be devoted entirely to course development and 2/3 of Shapere's Year 1 time will be spent on presentation and website development, with the remaining 1/3 spent on visits. In subsequent academic years, the co-PIs will spend half the allotted time preparing for and organizing visits and developing supporting materials, and half conducting the visits. The outreach program will be part of the State of Kentucky's contribution to the budget.

Three 3-year postdoctoral fellows will be supported, one for each of the 3 co-PIs. The postdoctoral fellows will collaborate with the co-PIs on the proposed research and assist in the education of supported graduate and undergraduate students. Das and Shapere's postdocs will be paid an initial base salary of \$43,000 per year. Gardner's will be paid at an annual salary of \$38,000 in Years 1-3 and be supported for 4.3 months of Year 3 (with the remainder to come from other sources). These salaries are commensurate with national norms in the Investigators' respective subfields.

Four graduate students will be supported as research assistants, and will work in collaboration with Das and Shapere and their postdocs on proposed projects. Their initial salaries will be \$ 18,313, the standard 12-month salary in the Physics Department at UK. Graduate student tuition for Year 1 is budgeted at \$4600 for each student on line G6, rising to \$5100 in Year 2 and \$5600 in Year 3. Two undergraduate students will be supported during the summer months of each of the 3 years, initially at \$3500 for two summer months of work.

Fringe benefits have been calculated as follows. FICA for the co-PIs, postdoctoral fellows and undergraduate students amounts to 7.65% of the salary. Other fringe benefits are at the rate of 1.0% of salary for postdoctoral fellows and undergraduate students and 3.0% of salary for the co-PIs. Retirement benefits for the co-PIs amount to 10% of the budgeted portion of their salaries. Health insurance for the PI and postdoctoral fellows are calculated at \$ 404.80 per month per person for the first year with a projected 10% increase for each subsequent year. Except where otherwise noted, salaries (and hence FICA) have been projected to increase at 4% per year.

The research described in this proposal will require extensive computational work. The work on phenomenology of black holes will involve intensive numerical and symbolic computations, while the work on holography will involve symbolic computations. In addition,

computers will be required for all personnel for word processing and electronic communication with remote collaborators. A heavy-duty color printer will be shared by the entire group and used for preparing presentations and publications and printing electronic publications (which dominate our field and contain an increasing number of color figures). We have thus requested three workstations at \$ 3000 each and a color laser printer at \$1500.¹ This equipment will be used at least 80% for project-related purposes.

The travel budget will fund travel to conferences and workshops and to DOE National Laboratories and other institutions for consultative visits, for Das, Shapere, the postdocs, and graduate students. Shapere and Das expect to attend at least 2 domestic conferences and 2 international conferences per year, attend workshops for up to one month per year, and make regular visits to major research centers. Postdocs will travel to an average of one domestic conference and one international conference per year, and will be encouraged to participate in workshops at major research centers. Graduate students will travel to one domestic conference and one summer school per year. Travel for Das and Shapere in Year 1 is budgeted at the rate of \$5500 per year each, for each of the postdocs at \$2500 per year, and for graduate students at \$1500 per year, increasing by 5% in each subsequent year.

Materials and supplies of \$5000 in Year 1 (with a 5% increase in each subsequent year) will cover data processing supplies, duplication costs, and long-distance telephone charges for Das, Shapere, the postdocs, and visitors (at \$50/month each).

Consultant Services funds will support a program of regular visits of 2 to 7 days by researchers from around the world, as well as a limited number of longer-term visitors. We plan to host 12 short-term visitors per year at an average cost of \$1000 per visit (increasing by 5% in each subsequent year). The remainder of the consultant services funds will support a series of longer-term visits of between one week and one month. The funds allocated in Years 1, 2, and 3 for longer-term visits are \$2154, \$4311, and \$19711. In Year 3, we plan to partially support a one-semester sabbatical visitor with these funds.

As a subcontractor through NKU, Prof. Fernando will receive some of her summer salary and benefits from the grant (Year 1: \$5202; Year 2: \$5636; Year 3: \$6069). NKU will contribute all associated indirect costs to the project, at the rate of 29.8%.

The University of Kentucky will contribute substantial matching funds to the proposal. In addition to the salary matching and teaching reduction mentioned above, UK will contribute the entire indirect costs of the project, at the rate of 47.0% for Year 1 and 47.3% for subsequent years. UK's total matching contribution for the 3-year period will be \$775,612.

¹These items are normally treated as indirect items by the University of Kentucky. However, due to the special nature of this project these items are being requested as direct costs.

Kentucky DOE EPSCoR Program

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Kentucky DOE EPSCoR Program

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Experimental Program to Stimulate Competitive Research

December 16, 2002

Dr. Matesh Varma
United States Department of Energy
19901 Germantown Road
Germantown, Maryland 20874-1290

Dear Dr. Varma:


On behalf of Kentucky's Governor, Paul E. Patton, and the Kentucky Statewide EPSCoR Committee, I wish to express our support for the attached proposal to the U.S. Department of Energy's EPSCoR Program. DOE's EPSCoR funded initiatives have had and continue to have important impacts in Kentucky and worldwide.

For example, using DOE EPSCoR support, instrumentation was developed and led to technology that is being used by the United Nations to locate dangerous landmines and by the European Union to identify hidden chemical agent weapons. Research in nano- and micro-technologies is providing new avenues for miniaturizing electronics, detectors and electromechanical actuators, the basis for which is in fundamental materials science. These and other DOE EPSCoR initiatives provide unique opportunities to Kentucky for developing world-class research and energy-related infrastructure.

Energy research is one of five priority focus areas legislated within the Commonwealth's New Economy Strategy. Accordingly, the Statewide EPSCoR Committee has voted to increase by 50% its budget this year for DOE EPSCoR related research. This is extraordinary in a tight fiscal year.

We hope that this attached proposal can be funded as it represents another critical step in building infrastructure for both Kentucky's academic institutions and economic future.

Sincerely,



Wimberly C. Royster, Chair
Kentucky Statewide EPSCoR Committee

Statewide EPSCoR Office
Kentucky Science and Technology Corporation
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Equal Opportunity Corporation

Kentucky DOE EPSCoR Program

Program Overview

The Kentucky DOE EPSCoR Program encompasses two research clusters and an overall management function. This approach continues from the first three years of the DOE EPSCoR Implementation Grant because both clusters have produced broad impacts and steady improvements in competitiveness. The Materials Research Cluster is entitled *Integrated Material Architectures: From Nanoscale Studies to Nano/Micro-Device Development*; the High Energy Research cluster is entitled *High Energy Theoretical Physics*.

The goal of our Program is to raise the profile and productivity of energy research and education in Kentucky to levels of national and international prominence and competitiveness. This goal is approached through specific research, education and outreach activities.

In Materials Research, the team effort between the University of Louisville and University of Kentucky, along with DOE national laboratories and industry, combines theoretical and experimental techniques. The team focuses on the understanding of fundamental issues that control the properties of carbon-based and silicon-based quasi-one dimensional nanostructures (Q1DNSs); and the design and development of microelectronic and MEMS-based devices and systems for environmental, industrial and biomedical sensing.

In High Energy Research, the team effort explores and elucidates theoretical and phenomenological aspects of elementary particles, quantum gravity and string theory. The team focuses on establishing strong cooperative and collaborative ties with leading national and international laboratories for high-energy physics research; the suitability of the University of Kentucky as a site for a planned Center for High Energy Theoretical Physics; and diverse educational and scientific appreciation opportunities for students, teachers and the general public.

The Kentucky DOE EPSCoR Program is managed by the Kentucky DOE EPSCoR Subcommittee. Its nine members represent five universities and two industries. Through its director, Dr. John M. Stencel, energy-related research and education initiatives are coordinated and linked to the DOE, the Commonwealth of Kentucky, participating universities, and the Kentucky EPSCoR governing body - the Statewide EPSCoR Committee. The Subcommittee also disseminates information and progress reports, promotes the building of energy research infrastructure through national and state agencies and industries, and cooperates with EPSCoR programs and personnel throughout the US.

The Kentucky DOE EPSCoR Program strives to achieve sustainable and nationally competitive research throughout the Commonwealth. Continuation of its funding through the next three years in both clusters is key to healthy and growing energy research initiatives in Kentucky.

INTEGRATED MATERIAL ARCHITECTURES: FROM NANOSCALE STUDIES TO NANO/MICRO-DEVICE DEVELOPMENT

I. RESEARCH CLUSTER OVERVIEW

The Kentucky DOE Materials Research Cluster is an integrated group of investigators emphasizing critical Department of Energy research goals in two major “focus areas” related to nanotechnology and MEMS (microelectromechanical systems). The first focus area concentrates on the fundamental studies of nanoscale materials to assess their potential towards nanoscale device development, while the second complementary focus area strongly emphasizes device applications through the use of nanoscale materials, implementing MEMS and microtechnology as “enabling platforms”. An interdisciplinary collection of key researchers from both the University of Louisville and the University of Kentucky has been assembled and appropriately grouped into two teams that will synergistically address the significant research challenges associated with each focus area. The two focus groups contain members with diverse but related backgrounds, and thus are capable of addressing the fundamental issues related to nanoscale materials as well as potential applications of these materials in fabricating nano/micro/mems-scale devices. The cadre of devices proposed in this research require the careful integration of several disciplines, including physics, chemistry, biology, mechanics, electronics, material science, MEMS and nanotechnology. The “fundamental science” group is primarily based in the physics discipline, and the “applications” group is predominantly from the engineering field. The two groups leverage the expertise and strengths of each other, interfacing regularly to discuss results and planned future directions. To enhance group interactions, each team contains, by design, a member whose educational background is from the others group’s primary focus area. For example, the “fundamental science” group contains one engineer, while the “applications” group contains one physicist. In this manner, the two groups remain integrated on a daily basis and are thus more sensitive to global issues of the research cluster. Focus Group A (the fundamental science group) is led by Dr. Chakram Jayanthi of the UofL Physics Department, and Dr. Kevin Walsh of the UofL Electrical and Computer Engineering Department heads the Focus Group B (the applications group).

Figure 1 presents an overview of the KY Materials Research Cluster and the thematic activities proposed in this research. The synergistic relationship between the two focus groups is represented by the interlocking puzzle in the background. The twelve individual research projects proposed by the cluster can be grouped into seven distinct thematic activities. As shown in the figure, six of those research themes surround a larger central figure symbolizing the common goal of the cluster for the development of novel nano/micro-devices for DOE applications. The location of the themes on the puzzle identifies the specific areas

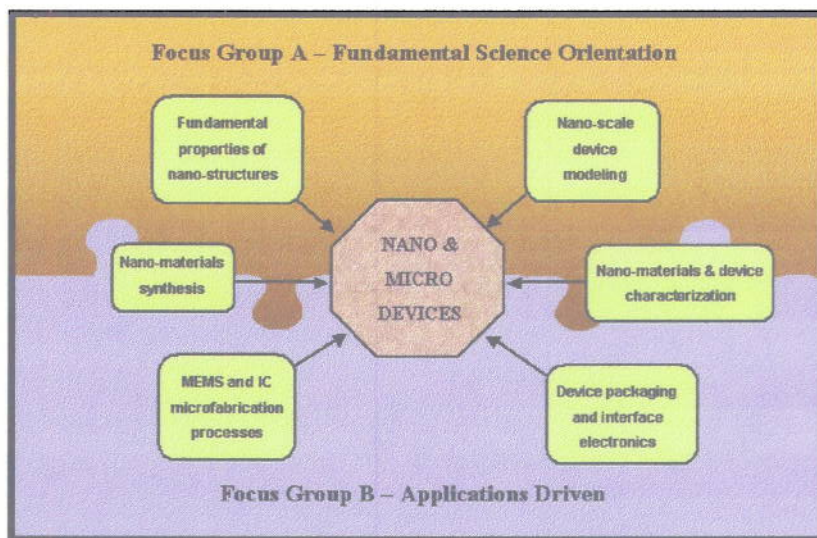


Figure 1. Thematic activities and interplay of the KY DOE EPSCoR Materials Focus Groups

of research of the two focus groups. Note that in two cases, the proposed research activities represent joint efforts, utilizing the combined resources of both teams. A summary of the research projects and educational programs proposed by each focus group appears below.

Focus Area A is concerned with the study of carbon-based and silicon-based quasi-one dimensional nanostructures (Q1DNSs). Q1DNSs are unique systems because of their nanoscale cross-sections and micrometer-scale lengths. This feature (high aspect ratio) leads to the transverse confinement of electrons, which, in turn, may endow a Q1DNS with unusual properties. Carbon nanotubes (CNTs) and silicon-based nanowires (SiNWs) have been chosen as case studies because of their potential as components in nanoscale devices. The scientific outcome will not only provide a fundamental understanding of the structural, electronic, transport, and optical properties of carbon- and silicon-based Q1DNSs, but also an assessment of the potential of these Q1DNSs for nanoscale device applications. Focus Group A is composed of six researchers who collectively have extensive experience in nanoscale materials research ranging from large-scale quantum mechanics-based simulations, to synthesis, to characterization, to fabrication. Our emphasis on a team approach, combining seamlessly experimental, theoretical, and fabrication techniques, is expected to result in the formation of a formidable and competitive team in materials research in Kentucky. Through the participation of post-doctoral fellows, graduate students, and undergraduate students in the emerging field of nanotechnology, the team will be training a cadre of next generation of engineers and scientists in this cutting-edge field. Focus Area A also includes an educational outreach program developed in collaboration with the Louisville Science Center (LSC). LSC serves the students and schools throughout the state of Kentucky through the Kentucky Tele-Linking Network (KTLN). Ms. Miller, a high school teacher at the Sacred Heart school, will be the coordinator for this program. She will be the liaison between our research group, the LSC, and the high school students. We will serve as scientific advisors to Ms. Miller and also provide the necessary technical and scientific expertise to the museum staff to create and maintain a permanent nanotechnology exhibit. Under Phase One DOE/EPSCoR funding, we have had very successful collaborations with Dr. Zhengyu Zhang of Oak Ridge and Dr. Meijie Tang of Lawrence Livermore, each leading to two high caliber publications. An additional collaboration has recently been established with Dr. Shawn-Yu Lin of Sandia, an expert in photonics, on device applications for silicon-based Q1DNSs. He is renowned for making the first photonic crystal. Most recently, Drs. Jayanthi and Wu have been invited to participate as research champions in key theoretical areas of nanoscale science for the newly founded Center for Nanophase Materials Sciences at the Oak Ridge National Laboratory.

Focus Area B will concentrate on application-driven solutions to selected DOE issues related to nanotechnology and MEMS-based microdevices and systems, as shown in Figure 1. The team of 6 researchers in Group B has an appropriate diverse background (EE, ME, bioengineering, MEMS, electronics, physics, chemistry and material science) and proven track record to effectively tackle the interdisciplinary issues involved in the design of such challenging solutions. Focus Area B has identified 6 specific projects of DOE interest, several of which are direct extensions of the research successes enjoyed during our Phase One DOE EPSCoR funding. All projects have the final goal of developing prototype nano/micro-devices for DOE-related sensing and/or electronic applications. Each of the six projects is of high DOE interest and collaborating DOE personnel and national laboratories (ORNL, Sandia, Argonne) are identified in the body of the proposal. The projects range from the study of molecular electronics using chemically-engineered nanoscale molecules, to MEMS-based micro-detectors using molecular science, to rugged high temperature ceramic microsensors implemented with ultra-precision micromilling techniques, to micro-total analysis systems using electrochemical detection, to custom wireless electronics for remote sensing applications. Furthermore, the proposed Group B research activities will be integrated into 5 existing technology courses currently offered in the engineering curriculum, thus exposing these research efforts to over 100 students a year, of which approximately 20% are female and/or minorities. Five graduate students and two research scientists will be directly supported by this Focus B DOE EPSCoR component. Additional educational outreach activities include: summer

internships in the cleanroom for undergraduates, annual laboratory tours to female minority high school students during Career Day for Women, and annual presentations to selected high school physics classes in Louisville. During the first 2 1/2 years of EPSCoR funding, the Group B Team has enjoyed much success with over 20 refereed publications, over 50 conference publications, 3 patents awarded, 7 patents pending, 14 additional external grants awarded (NSF, DoD, NASA, SwRI, NRL, KSTC, etc), and 6 grants pending.

Funding of this proposal will continue to enhance the already strong commitment that the state of Kentucky has reserved to research in the areas of advanced materials, nanotechnology and MEMS. It will also continue to enhance the state's commitment to building core infrastructure in these critical areas, as is evident by the construction of a new \$35M Science and Technology Building beginning in May of 2003 that will house an 8,000 sq. ft. class 100 Micro/Nano-Technology Cleanroom facility, which will rival those of Stanford, Berkeley and Cornell. That facility will permanently house the over \$5M of fabrication and characterization equipment that the two groups have successfully acquired over the last several years. This proposal continues those strong efforts.

II. RESEARCH CLUSTER FOCUS AREAS

A description of the two research focus areas appears below, along with their individual project descriptions, progress reports, DOE interactions, results, and educational opportunities.

A. FOCUS AREA A - *A Comprehensive Study of Carbon-based and Silicon-based Quasi-One-Dimensional Nanostructures: From Fundamental Science to Device Applications*

A1. Abstract

An understanding of the structural and electronic properties of quasi-one-dimensional nanostructures (Q1DNSs) is crucial for the design and the ultimate realization of nano-scale devices. This renewal proposal focuses on *carbon-* and *silicon-based* Q1DNSs because the interplay between the unique geometry of a Q1DNS (high aspect ratio), the transverse-confinement of electrons, and the hybridization characteristics of the respective atom are expected to lead to novel properties for these Q1DNSs. Specifically, this proposal focuses on the fundamental properties of *double-wall* carbon nanotubes (DWCNTs), silicon nanowires, and Si/SiGe superlattice nanowires and their device applications.

The proposal contains six projects, four of them devoted to DWCNTs and two to silicon-based nanowires. DWCNTs are interesting because they not only can serve as prototypes for multi-wall carbon nanotubes, but also are important nano-materials in their own right. **Project 1** aims at understanding how the composition of a DWCNT and its inter-shell interaction affect the transport properties of the DWCNT. **Project 2** concerns the modeling of an electro-mechanical switch based on a DWCNT. **Project 3** examines the feasibility of a DWCNT-based metal-semiconductor junction diode. **Project 4** studies a DWCNT-based metal-semiconductor field effect transistor (MESFET). **Projects 5 and 6** are devoted to nanowires. Specifically, **Project 5** focuses on the dependence of structural, electronic, and optical properties of silicon nanowires (SiNWs) on the diameter and orientation. **Project 6** concentrates on the study of the structural, electronic, and optical properties of Si/SiGe superlattice nanowires. The scientific outcome from the proposed projects is expected to provide a comprehensive understanding of the effect of interplay between the quantum confinement, the dimensionality, and the bonding nature on the properties of carbon- and silicon-based Q1DNS. It will also provide the platform to assess their potential as nano-scale inter-connectors, components for nano-scale electronic and electro-optical devices. To accomplish the work outlined in the proposal, a cross-disciplinary research team composed of two computational condensed matter physicists (Dr. Jayanthi and Dr. Liu), an electrical engineer (Dr. Chen from University of Kentucky), an experimental condensed matter physicist (Dr. Sumanasekera), and two condensed matter theorists (Dr. Wu and Dr. Yu) has been assembled. This team collectively has

experience in synthesis, electrical and optical characterizations, device modeling and device fabrication of carbon- and silicon-based nanostructures.

The proposal also contains an educational outreach program. This program is developed in collaboration with the Louisville Science Center (LSC). Ms. Miller, a Sacred Heart high school science teacher, will be the liaison person between our research group, the Louisville Science Center, and the high-school students from the Louisville Metropolitan area. The program consists of two parts. (1) We will provide the technical/scientific advice as well as resources to Ms Miller and the museum staff for creating and maintaining a cutting-edge nanotechnology exhibit at the museum. (2) Through the Kentucky Tele-Linking Networking facility at the museum that serves high schools in the Louisville metropolitan area, we will disseminate the educational program on nanotechnology to aspiring students and teachers. LSC also has a very active VOLUTEEN (volunteer-teen) program. Ms. Miller and the museum staff will train these teen volunteers in conducting some of their educational programs.

A2. Progress Report (Focus Group "A")

The research activities of Dr. Jayanthi and Dr. Wu under the DOE/EPSCoR award *DE-FG02-00ER45832* in the last two years have focused on the fundamental properties of silicon-based and carbon-based nanostructures using theoretical techniques developed at the University of Louisville, namely, an order-N non-orthogonal tight-binding molecular dynamics (O(N)/NOTB-MD) [A1,2] scheme for large-scale simulations and a local analysis technique [A3-5] for interpreting the properties of the system at a fundamental electronic or atomic level. The properties of nano-structures studied include the electronic, electro-mechanical, transport, and magnetic properties of single-wall carbon nanotubes (SWCNTs) and other related structures such as carbon nanotube rings. We have also investigated the electronic and optical properties of silicon clusters and Si_nGe_m nanoclusters, structural and mechanical properties of silicon nanorods, and the energetics of Si and Ge ad-atoms on Si(100) surface. These activities have resulted in 14 refereed publications (1 *Nature*, 3 *Physical Review Letters*, 3 *Physical Review B*, 1 *Phys. Reports*, 1 *J. Appl. Phys.*, 1 *Chem. Phys. Lett.*, 1 *J. Chem. Phys.*, 1 *Surf. Sci.* etc) with 3 other manuscripts under review, as listed in the bibliography section [A2, A6-A21], ~10 invited talks by PI/Co-PIs and ~10 contributed talks by post-docs/students at professional meetings. Our *Nature* and PRL articles [A7,A8] on the electro-mechanical effects and transport properties of SWCNT have already received several citations and our PRL article on the colossal paramagnetic moments in metallic carbon nanotori [A18] has been highlighted in the Physics web news by the editor, Ms. Katie Pennicott, as follows: "*Carbon nanotube bent into rings are the latest nanostructures to display surprising properties, according to new calculations. Shi-Yu Wu of the University of Louisville and colleagues found that the magnetic moments of some metallic nanotori were thousands of times stronger when the rings had certain magic radii*" (see, May 2002 issue: <http://physicsweb.org/article/news/6/5/13/1>). We collaborated with the experimental group headed by Prof. H. Dai (a pioneer in the carbon nanotube field) and Prof. R.B. Laughlin (1998 Nobel Laureate in Physics) of Stanford University, and Dr. M. Tang of LLNL in our research on the electronic and transport properties of metallic single-wall carbon nanotubes [A7-8, A14]. In our research on the growth structures of Si and Ge adatoms on a Si(100) surface, we collaborated with Dr. Z. Zhang (a leading surface physicist) of the Oak-Ridge National Laboratory [A16].

Two selected results relevant to the present proposal are summarized. In our studies on electro-mechanical effects of a metallic single-wall carbon nanotube, we found the electrical conductance to decrease by *two* orders of magnitude when a metallic single-wall carbon nanotube was pushed by the tip of an atomic force microscope by a small bending angle ($\sim 14^\circ$), due to the tip-induced sp^2 to sp^3 transition in the region of deformation of SWNT, with the process reversible when the tip was retracted. This result is significant because of its implications in the fabrication of nanoscale electro-mechanical switch.

Most recently, we have discovered that the interplay between the toroidal geometry and the ballistic motion of the π -electrons leads to colossal paramagnetic moments in metallic carbon nano-toroids formed from carbon nanotubes when a small magnetic field is applied. This result may be exploited in the fabrication of nanoscale magnetic sensors. This work forms the basis of one of our recently funded NSF/ECS proposal on "Carbon Nanotube based Spin Electronic Devices". Our research team also enjoys the support from the Division of Materials Research of the NSF on a grant entitled " Large-Scale Quantum Mechanical Molecular Dynamics Simulations: Challenges, New Directions, and Applications to Carbon-Based Nanostructures".

An Estimation of Unexpended Funds: We estimate approximately \$5,200 of DOE, \$7,680 of the state, and \$0 of the local funds may remain unexpended at the end of June 2003. They all pertain to the salary pool. This unexpended fund is mainly due to the 4-months phase lag between the actual start of the grant and the funding cycle.

Changes Affecting the Original Research Endeavor: The original proposal (DE-FG02-00ER45832) was primarily fundamental properties of carbon-based and silicon-based nanostructures using theoretical and computational studies. The current proposal includes experimental studies as well as device applications of nanostructures. We have therefore inducted 4 new members into our team, whose research backgrounds can help achieve the expanded scope of the proposal. Dr. Sumanasekera (UofL) is an experimentalist with research experience in synthesis (PLV, CVD, and PLA) and characterizations (electrical, optical, thermal, and thermo-gravimetric techniques) of carbon nanotubes and silicon nanowires [A22-A24]. He has successfully synthesized DWCNTs by annealing peapods [A24]. Dr. Chen is an Electrical Engineer from University of Kentucky. His research interest focuses on fabrications of carbon nanotube-based electronic devices, MOS transistor reliability and integrated micro/nano-scale sensors and microcircuits. Dr. Chen has successfully synthesized highly ordered and vertically aligned MWCNTs on *silicon substrates* using Al_2O_3 nanostructures as templates and the ethylene-flame synthesis method [A25-28] for their potential use in chemical gas sensors and transistors. The third new member, Dr. Liu, is an expert on the electronic and transport properties of single-wall carbon nanotubes and has made several outstanding contributions to this field. The fourth member, Dr. Yu is a female scientist, whose field of expertise is in the first-principles electronic structure calculations and optical properties of silicon-based nanoclusters and nanowires. The other significant change to the renewal proposal is that Dr. S. Liu and Dr. Sinnott are no longer part of this team. Dr. Sinnott left the University of Kentucky during the first year itself. However, we completed the original proposed project on "the thin-film nucleation through molecular beam deposition" in collaboration with her that resulted in a publication in J. Chem. Phys [A17].

A3. Introduction to proposed Projects - Focus Group "A"

Motivation: Quasi-one-dimensional nanostructures (Q1DNSs) such as nanotubes or nanowires have nanoscale cross-sections and micrometer lengths along the axial direction (*i.e.* high aspect ratio). This unique geometry of a Q1DNS leads to the confinement of electrons in the transverse direction and, hence, presents the opportunity for a Q1DNS to exhibit novel properties and phenomena. It is now becoming increasingly evident from the multitude of available experiments that Q1DNSs such as carbon nanotubes (CNTs) and silicon nanowires (SiNWs) will play a pivotal role in nanoscale electronics and optoelectronics, both as functional components and interconnects [A29-45]. While these experiments demonstrate novel device concepts based on SiNWs and CNTs, *there are still many critical issues that need to be clarified* before SiNW- or CNT-based electronic and optoelectronic devices can be routinely fabricated and their potential applications realized.

Double-Wall Carbon Nanotubes (DWCNTs): While the structural and the electronic properties of ideal single-wall CNTs (SWCNT) are reasonably well understood, not much is known about structures and

properties of multi-wall CNTs (MWCNTs). It is experimentally difficult to prepare a sample of well-defined and structurally characterized MWCNT [A46]. The knowledge on MWCNTs is still limited to the measurements of transport [A47-50] and mechanical properties [A51]. Theoretical study of MWCNTs, on the other hand, have been hampered by the fact that it is difficult to treat polychiral MWCNTs that are incommensurate (IC) with a lattice mismatch between the inner and outer shells [A52-54]. Recently, double-wall CNTs (DWCNTs) with a narrow distribution of diameters (~ 1.5 nm) were prepared from carbon peapods by the heat treatment [A24,55-57]. The controlled preparation of DWCNTs provides the opportunity to use them as prototypes for understanding how properties of MWCNTs depend on their composition and the intershell interaction. Furthermore, it also allows the exploration of the feasibility of developing DWCNT-based devices.

Silicon-based Nanowires: The feasibility of utilizing SiNWs in nanoscale electronic and optical devices is now apparent. However, a fundamental understanding of how the electronic and optical properties depend on the size and the orientation of SiNWs is still lacking. This information is crucial for the design and the fabrication of SiNW-based devices with desired properties. Very recently, there is an exciting report on the modulated growth of Si/SiGe nanowires with a superlattice structure [A58]. Thus there is the prospect of imposing an artificial periodicity along the axial direction of a Si-based NW by modulated growth of consecutive segments of Si component and Ge component of prescribed lengths (Si_mGe_n superlattice NWs, with m and n indicating the periodically repeating number of Si and Ge sections). This possibility opens an entirely new avenue to investigate the likelihood of creating a Si-based Q1DNS with a direct band gap.

Objectives: This proposal is a team effort that synergistically combines the *theoretical* and *experimental* techniques to understand the fundamental issues that control the properties of *carbon-* and *silicon-based* Q1DNSs for fabricating nano-scale devices. The nanostructures and the properties to be studied in this proposal include DWCNTs, SiNWs, and Si/Ge superlattice NWs and their structural, electronic, transport, electro-mechanical, and optical properties. The nanoscale devices to be studied include DWCNT-based metal-semiconductor junction, DWCNT-based MESFET, and DWCNT-based electro-mechanical switch. Several questions critical to the design of nano-scale devices will be addressed. For example,

- *How do the composition, the commensurability between the inner and outer shells, and the inter-shell interactions of a DWCNT affect its transport properties?*
- *How do the structural, electronic, transport and optical properties of a SiNW vary as a function of its diameter, its orientation and its surface modification?*
- *How to controllably synthesize DWCNTs and Si/Ge superlattice Q1DNSs?*

Background on Theoretical Techniques: The structural determination of nanostructures will be carried out mainly using the O(N)/NOTB-MD scheme [A1], as DFT-based molecular dynamics scheme are beyond the scope of available computer resources. In situations where charge-transfer becomes important, we will use a more accurate SCED-LCAO semi-empirical Hamiltonian, where the electron-ion and electron-electron interactions are modeled in a manner that closely mimics the first-principles Hamiltonian. Since this Hamiltonian is built in the framework of linear combination of atomic orbitals (LCAO) with multi-center interactions modeled via environment-dependent (ED) terms and the charge density determined self-consistently (SC), we refer this Hamiltonian as a SCED-LCAO Hamiltonian. Molecular dynamics codes corresponding to this Hamiltonian have been developed by the Louisville group [A59].

Background on Synthesis Techniques: Peapods are SWCNT-based hybrid materials with fullerenes encapsulated in SWCNT [A60-62]. Recently DWCNTs with a very narrow distribution of diameters have been produced by heat-treating peapods at 1200 °C or above, leading to the coalescence of the encapsulated C_{60} 's and the subsequent formation of a NT inside the primary (outer) NT [A24, 55-57].

In this proposal, Dr. Sumanasekera will first synthesize SWNTs in his laboratory in bulk quantities using conventional pulse laser vaporization (PLV) [A64] and chemical vapor deposition (CVD) [A65] techniques. The pristine material will be purified using selective oxidation followed by mild acid treatment. Then the purified material will be heated in dry air at appropriate temperature to open the tubes, which is crucial for the diffusion of C_{60} inside the SWNTs. This can be accomplished by maintaining C_{60} vapor at elevated temperatures along with the SWNTs (open) in an evacuated and sealed glass ampoule. DWNTs will be prepared by annealing the peapods at 1200 °C in high vacuum ($<10^{-6}$ Torr) [A24].

A4. Proposed Research

This section identifies specific tasks on DWCNTs and silicon-based NWs to be carried out in this proposal that are critical to the design of nano-scale devices based on these structures.

Project 1 Transport Properties of Small-Diameter DWCNTs

DWCNTs are interesting not only because they can serve as prototypes to study properties of MWCNTs in general but also because they are promising nano-materials in their own right [A63]. For small-diameter DWCNTs produced from peapods, the diameter of the outer shell is ~ 1.4 nm while that of the inner shell is ~ 0.7 nm. The size of these DWCNTs, though still very large, is however well within the range of capability of our theoretical tools (the $O(N)$ /NOTB-MD scheme and the method of real space Green's function). Thus the existence of the small-diameter DWCNTs offers a rare opportunity to investigate properties of complex systems with both theoretical and experimental tools on equal footing.

Transport measurements on MWCNTs have indicated that their transport behavior can range from ballistic to quasi-ballistic or diffusive but with low resistance if the MWCNT has at least one metallic shell [A47-A50]. However, because it is difficult to prepare a sample of well-defined and structurally characterized MWCNT [A46], the understanding of the system properties of MWCNTs is still lacking. Key features affecting transport properties of a MWCNT include its composition, the commensurability of the translation vectors of its constituent shells, and the intershell interaction [A66]. These features can be readily studied in the case of small-diameter DWCNTs.

Theoretical Investigations (*Wu, Jayanthi and Liu*): We plan to systematically investigate the transport properties of four classes of defect-free DWCNTs. They include (i) commensurate (C) metal@metal, (ii) incommensurate (IC) metal@metal, (iii) semiconductor@metal, and (iv) metal@semiconductor. Our strategy will start with the determination of the structure of the DWCNT $(n_i, m_i)@(n_o, m_o)$ using the $O(N)$ /NOTB-MD scheme [A1] based on the NOTB Hamiltonian developed by Menon and Subbaswamy [A67]. With the structure of the DWCNT determined, we will then calculate the electrical conductance using the Landauer formula [A68] with the inter-shell interaction modeled by a tight-binding (TB) Hamiltonian and with the electrode contacts assumed to be attached to the outer wall of the DWCNT. The conductance of DWCNTs with lengths up to tens of nanometers is possible if the real-space Green's function method [A69] is used to calculate the transmission coefficients appearing in the Landauer's formula of conductance. The method also provides a convenient scheme to calculate the local electronic density of states (LDOS) that is essential to obtain a detailed picture of the electronic structure. We will analyze the conductance with respect to the composition of the DWCNT, the commensurability between the inner and the outer walls, and the nature of the outer wall where the electrode contacts are made to gain a complete picture of how these factors affect the electrical conductance.

Experimental Investigations (*Sumanasekera*): DWCNTs prepared in our laboratory will be dispersed in Dimethylformamide (DMF) by ultrasonic agitation and spin coated on to a thermally oxidized,

degenerately doped Si substrate which will have pre-defined alignment marker grids. We will map out and record the DWCNTs with respect to these alignment marks using an atomic force microscope (AFM). First the sample will be studied using micro-Raman to identify the chirality of the inner and the outer tube of identifiable DWCNTs (with respect to the alignments marks) by studying the radial breathing mode (RBM) [A24]. Dr. Sumanasekera will use the micro Raman facility at the Pennsylvania State University for this part of the investigation. Next, for electrical transport studies, contact patterns will be defined using e-beam lithography, again identifying the DWNTs with respect to the alignment marks. Au/Ti evaporation followed by lift-off will be used to make contacts over the respective DWCNTs. The e-beam lithography defined contacts will be attached to larger areas of optical- lithography defined pads, and the device will be wire-bonded and packaged. The e-beam lithography and optical-lithography facilities available at the University of Louisville will be used for this part of the work.

We will perform both two-point probe and four-point probe measurements on the DWCNTs. With the two-point probe measurements, we will be able to study interesting properties, especially when the outer tube is semiconducting as it forms a Schottky barrier with the metal contact. Two-point I-V characteristics should reflect the modification of Schottky barrier properties due to interplay between inner and outer tubes. This can be compared to the properties of a Schottky barrier created with an individual semiconducting SWNT and a metal contact. But two-point probe measurements will not directly give the 'intrinsic' resistance of the DWCNT. Therefore, four-probe resistance measurements will be performed to extract the intrinsic resistance of the DWCNT. Furthermore, this will allow us to extract the value of the contact resistance too. The measurements of the contact resistance at the schottky barrier (in the case of semiconducting outer tube) should again provide valuable information about the interplay between the inner and outer tubes. We will also perform *in situ* annealing and doping (both n-type and p-type) of the device. This will allow us to study the doping effect on the DWCNTs. In fact in the case of air-stable doping conditions, we will go back and re-measure the Raman properties of respective DWCNTs.

Scientific Outcomes: This synergistic approach of studying the transport properties of a DWCNT is expected to not only shed light on the physics behind the transport behavior of those DWCNTs with at least one metallic shell but also to provide an understanding of the effect of the tunneling across the shells on the transport behavior. Indeed, a DWCNT presents an unique opportunity to probe the role of the inter-shell interaction on the conductance particularly to decipher if the channels associated with the inner NT become accessible for the conduction process.

Project 2 Electro-Mechanical Properties of a DWCNT: A Prototype Nanoscale Switch?

Motivation for studying Electro-mechanical Effect in a DWCNT: In our previous studies on the interplay between the mechanical deformation and the electrical properties of metallic SWCNTs [A7,8], we have found that a *local* deformation induced by an AFM tip can cause a dramatic and reversible two orders of magnitude reduction in the conductance at relatively small bending angles ($\sim 14^\circ$). This demonstration of the electro-mechanical effect in a SWNT indicates strongly the potential for using CNTs as a component for nano-scale electro-mechanical switching devices. However, to realize this potential requires the enhancement of this effect by at least another order of magnitude.

For a DWCNT, factors affecting the interplay between its mechanical deformation and electrical properties include (i) the commensurability between its inner and outer shells, (ii) the inter-shell interaction, (iii) the proximity between the inner and outer shells (~ 0.34 nm) and, in the case of small diameter DWCNTs, the smallness of the diameter of the inner shell (~ 0.7 nm), and (iv) the stiffness and the toughness of small-diameter DWCNTs. Thus a combination of a number of these factors may enhance the interplay between the local mechanical deformation and the electrical properties in small-diameter DWCNTs. Therefore we propose to carry out an in-depth theoretical and experimental study of the local

deformation of DWCNTs by an AFM tip to determine the feasibility of enhancing the reversible reduction of the conductance exhibited by a metallic SWCNT by one *more* order of magnitude.

Theoretical Investigations (Jayanthi, Liu and Wu): We plan to follow a similar approach as we have used previously in the study of the local deformation of SWCNTs [A8]. We will focus our attention to three classes of DWCNTs, namely, commensurate metal@metal, incommensurate metal@metal, and semiconductor@metal. We will start our investigation by first conducting a careful modeling of the continuous pushing action of an AFM tip against the DWCNT under consideration, using our O(N)/NOTB-MD scheme [A1]. During the simulation of the continuous pushing action of the tip against the DWCNT, we will monitor the structure of the DWCNT, in particular, in the immediate vicinity of the tip, to detect any topological change in the structure of DWCNT. Once such a change is observed, we will carry out a local analysis [A5] to determine whether there is a change in bonding structure from the sp^2 to sp^3 bonding configuration and also determine the extent of the region of change. We will also examine whether the structural and bonding changes are reversible as the AFM tip is withdrawn from the DWCNT. Finally, we will calculate the conductance of the DWCNT under the local deformation induced by the AFM tip based on the Landauer's formula, using the real space Green's function [A69]. We will calculate the conductance for different compositions of DWCNTs outlined above and analyze the result in terms of change in the local electronic properties to provide insight into the feasibility of a DWCNT-based electro-mechanical switch based on the best case scenario for conductance change.

Experimental Investigations (Sumanasekera): We will follow the same procedure as described in project #1 in preparing the samples. In addition, we will create series of trenches (~ 200 nm wide and ~ 200 nm deep) on the Si/SiO₂ substrate (containing alignment marks) using ion etching prior to dispersion of the DWCNTs. The DWCNTs bridging the trenches will be identified and mapped out using pre-defined alignment grids and studied for chirality by micro-Raman. *In situ* conductance will be measured (by making the contacts as in project #1 by depressing the DWNT using an AFM tip [A7,8]).

Scientific Outcomes: The result of the combined theoretical and experimental investigation of the local deformation of DWCNTs is expected to provide a detailed picture of the effects of factors such as the composition of the DWCNT, the commensurability of the inner and outer walls, the possible transition from the sp^2 to the sp^3 bonding configuration, the proximity of the inner and outer walls, and the smallness of the inner NT on the interplay between the mechanical deformation and the electrical properties of DWCNTs. Our assessment of the likelihood of enhancing the reduction of the conductance using a DWCNT under the manipulation of a local probe could lead to the realization of a prototype of nano-scale switch, indeed an important advancement in the fabrication of nano-scale electro-mechanical devices.

Project 3 DWCNT-Based Metal-Semiconductor Junction

A Novel Device Concept: It is straightforward to conceive a metal-semiconductor junction based on a DWCNT of either a semiconductor@metal or a metal@semiconductor type. For example, by pulling the inner shell with respect to the outer shell of the above-mentioned DWCNT by a certain length using a nano-manipulator, a metal-semiconductor junction with the interface defined by the overlap between the inner and outer SWCNTs can be created. The experimental procedure for telescope-like sliding movement by pulling inner shells with respect to outer shells of a MWCNT using a nano-manipulator has been reported by Zettl *et al.* [A70] They have also reported a procedure for peeling off the shells of a MWCNT [A71], which will be exploited in this proposal to create a DWCNT-based device (see Fig. A1).

Theoretical Investigations (Jayanthi, Wu and Liu): The theoretical calculation involved in this project, while tedious, is comparatively straightforward. We will calculate the current as a function of the bias (forward as well as reverse) voltage at a fixed overlap length between the outer and inner SWCNT.

Within the framework of the model tight-binding Hamiltonian used to describe the electronic structure of the CNT, the potential across the overlap (interface) can be approximated by a linear function of the distance along the tube axis because of the magnitude of the bias voltage. The resulting I/V characteristics can then be used to determine whether this junction possesses the rectifying property. We will also study the I/V characteristics for various overlap (interface) lengths to assess its effect on the transport across the junction. If the calculations reveal the inadequacy of the linear approximation of the potential across the junction, we will implement the self-consistent and environment dependent LCAO-based (SCED-LCAO) Hamiltonian developed by our group [A59] to self-consistently determine the potential across the junction.

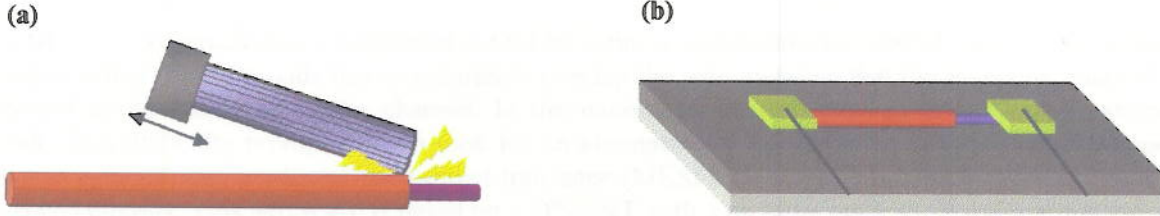


Fig. A1. (a) A nano-manipulator (gray) attached to a MWCNT is used to create a DWCNT-based device where part of the outer shell (red) of a DWCNT is removed to expose the inner shell (purple); (b) A DWCNT electrically contacted to its outer and inner shells to create a metal-semiconductor junction.

Experimental Investigations (Sumanasekera): The experimental procedure of this project, however, is very demanding. Two difficult aspects of the experimental investigation require particular attention. (1) The creation of a DWCNT-based metal-semiconductor junction. (2) The effect of the additional Schottky barrier between the semiconducting CNT and the metal contact. Pulling out the inner tube of a DWCNT is such a delicate procedure to render it unlikely at present. We therefore propose to follow an alternative procedure used by the Zettl *et al.* group in which the outer shells can be successively removed (peeling and sharpening) from a MWCNT [A71]. This will be done by an electrically driven vaporization of the outer tube. First we identify the chiralities of the DWCNT using micro-Raman and attach one end to a gold electrode. A longer multiwall nanotube attached to the nano-manipulator will be used as the shaping electrode. The DWCNT, with part of the inner NT exposed after removing part of the outer NT, will be carefully removed from the gold contact and laid on a Si/SiO₂ substrate to be used for electrical transport measurements. Au/Ti contacts will be defined over the DWCNT-based metal-semiconductor junction as described before. The I-V characteristics will be studied for the junction under different biasing conditions. In the case where the outer tube or the inner tube is semiconducting, our measurements will be plagued by the formation of an additional Schottky barrier at the semiconducting tube/metal contact junction. To overcome this situation, we propose to measure the property of a Schottky barrier formed by an individual SWNT with the metal contact. This will allow us to correct for the effect from the undesired Schottky barrier at the metal contacts and extract the properties inherent to the tunnel junction defined by the overlap between the two tubes of a DWCNT-based metal-semiconductor junction.

Project 4 DWCNT-Based Metal-Semiconductor Field-Effect Transistor (Chen, Wu and Jayanthi)

Avouris *et al.* [A72] recently reported an improved SWCNT field effect transistor (CNFET). The transconductance of the CNFET (p-channel) was found to be 2321 $\mu\text{S}/\mu\text{m}$, far better than that of the most recently fabricated p-type Si metal-oxide-semiconductor field-effect transistor (MOSFET) with a transconductance of 975 $\mu\text{S}/\mu\text{m}$ for the 15 nm gate Si p-MOSFET [A73]. We have estimated the hole mobility to be 2018 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ based on the reported data of the transistor structure. This value is much larger than the ideal hole mobility in bulk Si ($\sim 400 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$) and about 200 times higher than the hole

Theoretical Investigation (Yu, Jayanthi and Wu)

Structural Properties: To examine how the stability of a NW with its axis oriented along a *general direction* $\langle lmn \rangle$ depends on its diameter, we plan to carry out the energy optimization for the NW under study using our O(N)/NOTB-MD scheme [A1] because MD cells for NWs with diameters of ~ 20 nm contain $\sim 20,000$ atoms. In the simulation, we will choose the initial configuration for a SiNW with a given diameter and its orientation along $\langle lmn \rangle$ by cutting a cylinder of that diameter out of the bulk silicon with its axis aligned along the $\langle lmn \rangle$ direction. The MD cell composed of an appropriate number of atomic layers perpendicular to the $\langle lmn \rangle$ direction will be chosen with the periodicity imposed along $\langle lmn \rangle$. The stability issues pertaining to a SiNW of certain orientation and a certain diameter will be analyzed by examining the surface energy and surface structure so that issues related to the possible existence of the magic diameters and the critical size for growing straight single crystalline SiNWs may be understood. The effects of passivation on the structural properties of SiNWs will also be studied by conducting simulations with the dangling bonds on the surface of SiNWs passivated by hydrogen atoms.

Electronic Properties: With the relaxed stable structures of unpassivated and passivated SiNWs determined, we plan to calculate the total and local electronic density of states (TDOS and LDOS) of these NWs as a function of the diameter and the orientation, using the method of real space Green's function [A69] to handle the large number of atoms contained in SiNWs. The analysis of the TDOS and the LDOS as a function of the diameter and the orientation is expected to shed light on (i) how the energy gap depends on the diameter and the orientation of the NWs, (ii) how the gap states are related to the surface reconstruction of the unpassivated NWs, (iii) what effects does the passivation of the dangling bonds have on the gap states, and (iv) what are the nature of the gap states. The information is crucial for the design and fabrication of SiNW-based and doped SiNW-based electronic devices.

Optical Properties: The intense effort on the study of optical properties of SiNWs stems from the desire to improve the efficiency of the photoluminescence (PL) of this Si-based structure so that they can be seamlessly incorporated into prevailing Si-based electronics to create functioning optoelectronic devices. Two features of this Q1DNS are expected to play prominent roles in the design and the fabrication of SiNW-based optoelectronic device. They are the energy gap and whether the gap is a direct gap. The information concerning the tunability of the energy gap as well as the possible transformation from an indirect- (bulk) to a direct-band gap semiconductor for SiNWs as a function of the diameter and the orientation can be readily obtained from the analysis of the electronic structure. In addition, because quantum confinement is expected to cause an increase in the overlap between electron and hole states, we propose to calculate the radiative transition probability, a more fundamental quantity, to identify the factors responsible for enhancing the PL in SiNWs [A19]. This will allow us to assess the possibility of tuning the efficiency of the PL by changing the diameter and the orientation of SiNWs.

Experimental Investigation (Sumanasekera): Experimentally, we will synthesize SiNWs by pulsed laser vaporization (PLV) method [A74] using $\text{Si}_x\text{Fe}_{1-x}$ or $\text{Si}_x\text{Au}_{1-x}$ targets with appropriate stoichiometry. The orientation and the diameter of a NW will be determined by HRTEM. The orientation will be further confirmed by SAED, and XRD [A74]. We propose to perform electrical, optical and thermoelectric characterization of SiNWs. We will perform PL and optical absorption measurements for SiNWs with varying diameters and orientations to extract information about the energy gap and emission efficiency [A43,82,83]. Optical absorption will provide information about exciton processes and absorption edges of the NW [A84-86]. We will also measure the optical conductivity of individual NWs in a wide range of wavelengths to probe the carrier lifetimes and impurity states. We propose to measure the electrical conductivity (temperature and magnetic field dependence) and thermoelectric power of NWs to determine the band gap, majority carrier type, carrier concentration, and impurity concentration [A41].

Project 6 Structural, Electronic and Optical Properties of Si-based Superlattice Nanowires

Very recently, Wu *et al.* reported the growth of Si/SiGe superlattice NWs (SLNW) using a hybrid pulsed laser ablation/chemical vapor deposition (PLA-CVD) process [A58]. SEM images of these NWs indicate a diameter distribution from 50 to 300 nm. Periodic modulation of the structures was confirmed by the energy-dispersive X-ray spectroscopy. Although there is yet no systematic characterization of their structures and no measurements on their electronic and optical properties, the mere demonstration of creating Si/SiGe SLNWs with modulated periodicity suggests the possibility of controlled fabrication of Si/Ge SLNWs. If that possibility is realized, it opens the way to control the periodicity along the axial direction for Si-based Q1DNs, which in turn could lead to the creation of Si-based direct-band gap semiconductor NWs.

Theoretical Investigation (Yu, Jayanthi and Wu): Theoretically, we propose to carry out a detailed study of the structural, electronic, and optical properties of Si/SiGe SLNWs, using the same procedure as outlined in project 5. Our main goal is to gain an understanding of factors affecting the stability and the optical efficiency of these SLNWs in terms of their diameter, composition, and orientation to assess their potential in device applications. We also plan to conduct a similar study on Si/Ge SLNWs with the emphasis on assessing the feasibility of fabricating stable Si/Ge SLNWs and creating Si-based direct-band gap semiconductor SLNWs.

Experimental Investigation (Sumanasekera): Experimentally, we will first synthesize Si/SiGe SLNWs using the hybrid PLA-CVD method proposed by Wu *et al.* [A58]. Vapor-liquid-solid (VLS) mechanism will be initiated by introducing a mixture of H_2 and $SiCl_4$ (or SiH_4) at 850^0 - 950^0 C. During this process Ge vapor will be introduced into the liquid alloy intermittently by turning the laser on. By periodically turning laser on/off Si/SiGe SLNWs will be synthesized. For Si/Ge SLNWs synthesis, we will implement the following two methods. (i) Similar procedure will be used as in the case for Si/SiGe structure except for the fact that the SiH_4 flow too will be interrupted every time the laser is on. When laser is off, SiH_4 flow will be resumed. Periodic turning on/off of laser and SiH_4 flow can be easily programmed. (ii) Here we propose to make a composite target consisting half Si and half Ge and use only the PLV method (in the absence of CVD). Laser can be programmed to raster on Si part first for a pre-determined time and will be changed over to the Ge part and raster again for a pre-determined time. This will be done periodically.

We plan to measure the photoluminescence and optical absorption for Si/SiGe as well as Si/Ge SLNWs of varying modulation periodicity to study the band gap properties, using the procedures outlined in project #5. Recent renewed interest in the search for high efficiency thermoelectric systems has brought the attention to semiconductor superlattices. Already, some improvements in the thermoelectric figure of merit have been achieved for 2D transport in semiconductor SLs [A87]. We will measure the power factor ($S^2\sigma$ where S is Seebeck coefficient and σ is the electrical conductivity) of these SLNWs with varying modulation-periodicity.

A5. Broader Impacts of the Proposed Activity

Impact on Materials Research in Kentucky: University of Louisville already has a core group of researchers from Physics, Chemistry, Electrical Engineering, and Chemical Engineering working in the field of material science and nanotechnology. To further stimulate the inter-disciplinary research in material science and nanotechnology, a new research building (\sim \$35 M) housing researchers working in this area will soon be under construction. With the funding from federal agencies such as DOE/EPSCoR, we expect to build a first-rate research institute that advances the frontiers of material science and nanotechnology in Kentucky. For example, the collaborative efforts of Drs. Chen (University of Kentucky), Jayanthi, Sumanasekera, and Wu (University of Louisville) fostered in this proposal are

expected to result in the formation of a formidable and competitive team in Kentucky, capable of taking on challenging tasks in materials research in general and in nanotechnology in particular.

DOE National Laboratory Affiliations and Collaboration: Our research team has on-going research collaborations with the DOE National laboratories. Under the DOE/EPSCoR award DE-FG02-00ER45832, we have had very successful collaborations with Dr. Zhengyu Zhang of Oak Ridge National Laboratory (ORNL) and Dr. Meijie Tang of Lawrence Livermore National Laboratory (LLNL), each leading to two high caliber publications, including one in *Nature* and one in *Physical Review Letters*. For the renewal proposal, an additional collaboration has been established with Dr. Shawn-Yu Lin of Sandia on device applications of silicon-based Q1DNSs. Dr. Lin is an expert in photonics (*letter of support enclosed*). He is renowned for making the first photonic crystal. Most recently, Drs. Jayanthi and Wu have been invited to participate as research champions in key theoretical areas of nanoscale science for the newly founded Center for Nanophase Materials Sciences of the Oak Ridge National Laboratory. They will actively participate in the research activities of the nanomaterials theory group of this center.

Educational Activities: The PI and Co-PIs are committed to transfer their knowledge and experience to train students and postdocs in the emerging field of nanoscale science and engineering. Funds have been requested in this proposal for 2 graduate students and 1 post-doctoral fellow. Having a mix of junior and senior researchers is important in a scientific/technical field as junior researchers can learn/grasp quickly difficult research topics from the postdocs. At the same time, the mentorship-role assumed by the pos-doc provides them with a valuable professional experience. Furthermore, through the participation of undergraduate, graduate students, and post-doctoral fellows in the cutting-edge research, we will be training and building a cadre of the next generation of scientists and engineering in the exciting field of material science in Kentucky

Outreach Activities: In collaboration with the Louisville Science Center (LSC), we have developed an educational outreach program. Our outreach program consists of two parts. (1) We will provide the technical and scientific expertise to the museum staff to create and maintain a permanent nanotechnology exhibit. (2) We will serve as scientific advisors to the Tech Forum program of LSC, in particular in the development of a hands-on educational program in nanoscience. The outreach program will be coordinated by Ms. Nancy Miller, a science teacher at the Louisville Sacred Heart Academy. Ms. Miller will serve as the liaison person between our research group, the LSC, and the high-school students from the Louisville metropolitan area.

B. FOCUS AREA B – Applications of NanoScale Materials for the Development of Microelectronic and MEMS-based Devices and Systems

B1. Abstract

The Kentucky Materials “Group B Focus Team” leverages its success enjoyed from its prior 2 years of DOE EPSCoR funding and, in this 3-year renewal proposal, introduces 6 follow-on projects of high DOE interest. All projects involve nano-scale materials in one theme or another for the development of micro-sensors and single-molecular electronic devices. In the first project, entitled “Single Molecule Electronic Devices”, we investigate the use of chemically-engineered nanoscale molecules for the fabrication of ultra-high density circuits and extremely sensitive biological and chemical detectors. Single molecular electronic and spin-electronic devices should provide new functionality and an order-of-magnitude reduction in device size compared to the best possible efforts of silicon technology. The second project, entitled “Self-contained” μ TAS Devices with Electrochemical Detection”, is a direct continuation of our Phase One research where we integrate MEMS technology and microfluidics for the development of a lab-on-a-chip (LOC) device for the separation and analysis of inorganic species and small organic molecules for applications in environmental monitoring, industrial process control, and remote sensing.

The third and fourth projects represent a marriage of biomolecular science and MEMS technology. In these projects, MEMS will be used as the “platform” technology for the creation of microstructures onto which biological molecules are deposited. In project three, entitled “MEMS-based Multi-Species Fluid Analysis Device”, micro-calorimeters will be designed and fabricated with integrated flow channels for biomedical sensing applications related to DOE life science research interests. In project four, entitled “Bioelectronic MEMS Detectors for Chemical and Biological Warfare Agents”, MEMS technology and biology will again be combined to produce bioelectronic membrane sensors for the detection of nerve agents. Project five, entitled “Ultra- High-Precision Micromechanical Machining of Ceramic Materials”, utilizes the ultra-precision micro-milling/drilling technology acquired during our Phase One DOE funding for the development of high temperature ceramic-based microsensors for harsh industrial environments. And finally, in the sixth project, entitled “Telemetry Development for a Retinal Prosthesis”, we develop a wireless RFID communication platform, which can be used to interface remotely with microsensors, in general, and a retinal implant device specifically. All six projects are of high DOE interest and collaborating DOE personnel and laboratories (Oak Ridge, Sandia, Argonne) are identified in the proposal. Furthermore, the proposed research activities will be integrated into 5 existing micro/nano-technology courses currently offered in the engineering curriculum, thus exposing these research efforts to over 100 students a year, of whom approximately 20% are female and/or minorities. Five graduate students and 2 research scientists will be directly supported by this Focus B DOE EPSCoR component. Additional educational outreach activities include: summer internships in the cleanroom for undergraduates, annual laboratory tours to female minority high school students during Career Day for Women, and annual presentations to selected high school physics classes in Louisville. Funding of this proposal will greatly enhance the “advanced materials” research infrastructure in the state and leverage the already strong commitment that Kentucky has made to this critical area of research. This commitment is exemplified by the construction of a new \$35M Science and Technology Building beginning in May of 2003 that will house an 8,000 sq. ft. class 100 Micro/Nano-Technology Cleanroom facility, which will rival that of Stanford, Berkeley and Cornell.

B2. Introduction

The Materials Research Cluster is presently in its 3rd year of DOE EPSCoR funding. The core group of the Focus Area B Research Team has remained basically intact over that period and has consisted of Dr. Walsh (UofL ECE), Dr. Keynton (UofL ME), Dr. Baldwin (UofL Chem) and Dr. Naber (UofL ECE). During the first year of the grant, Drs. Grimes (UK EE), Dickey (UK Materials), Sinnot (UK ChE) and Mason (UK EE) accepted faculty appointments at Penn State, Penn State, Florida and Michigan, respectively and therefore had to be replaced. To fill the void left behind by their departure, the experimental team recruited Dr. Bruce Alphenaar, a new UofL University Scholar specializing in nanotechnology and molecular electronics with prior experiences at Yale, Hitachi and Cambridge University. To support Dr. Alphenaar’s research in nanotechnology, a subcontract was awarded to UK for the synthesis of carbon nanotubes (Dr. Rodney Andrews). The addition of Dr. Alphenaar allowed the Group B experimentalists to expand more heavily into specific areas of nanoscale materials, thus complementing more completely the companion efforts of the basic science group lead by Dr. Jayanthi. For the new research introduced in this proposal, the group is being further expanded with the addition of Dr. Bruce Hinds (UK Chem and Mat Eng), an expert in molecular electronics and nanoscale chemistry. Dr. Hinds enjoys an already active collaboration with Drs. Alphenaar and Walsh, which promises to be solidified with the funding of this proposal.

B3. Progress Report

During the first 2 1/2 years of funding, the Group B Team has enjoyed much success with over 20 refereed publications, over 50 conference publications, 3 patents awarded, 7 patents pending, 14 additional external grants awarded (NSF, DoD, NASA, SwRI, NRL, KSTC, etc), and 6 grants pending. Several of the successful devices that the team has developed during the first 2 1/2 years of funding under the DOE EPSCoR program appear in Figure A1. These range from selectively grown carbon nanotubes

on lithographically-patterned oxidized silicon in collaboration with UK, to numerous MEMS-based devices and systems for specific DOE applications fabricated directly in the UofL MicroTechnology Cleanroom. In addition, the group has been extremely successful in building critical infrastructure for nanotechnology and MEMS research in the state of Kentucky. As a result, the class 100 Microtechnology Cleanroom and supporting laboratories at the University of Louisville Lutz Hall now contains a full complement of design, processing and packaging equipment (~\$5M), allowing complete in-house solutions to custom prototype development for all researchers throughout the state of Kentucky. All necessary processes are available ranging from design and modeling using MEMCAD, to laser direct-write pattern generation for custom photomask fabrication, to deep reactive ion etching (DRIE) for MEMS development, to nano-imprinting for nanotechnology, to dicing and wirebonding for custom packaging. In addition, the state will begin construction next year on an 8,000 sq. ft. cleanroom facility (to be housed in the new \$35M Science and Technology Research Building) that will rival those of Stanford, Berkeley and Cornell, thus positioning the research universities in Kentucky in a competitive position to attract additional external funding, consistent with the goals of the EPSCoR program. The research and infrastructure presented in this proposal continues the excellent commitment made to Materials Research in the state of Kentucky, which dovetails perfectly with the interests of the Materials Science and Engineering Program at the DOE. It is anticipated that the equivalent of 4 months of salaries and fringe will remain at the end of 2002 June due to the 4 month phase lag between the actual start of the award and the funding cycle.

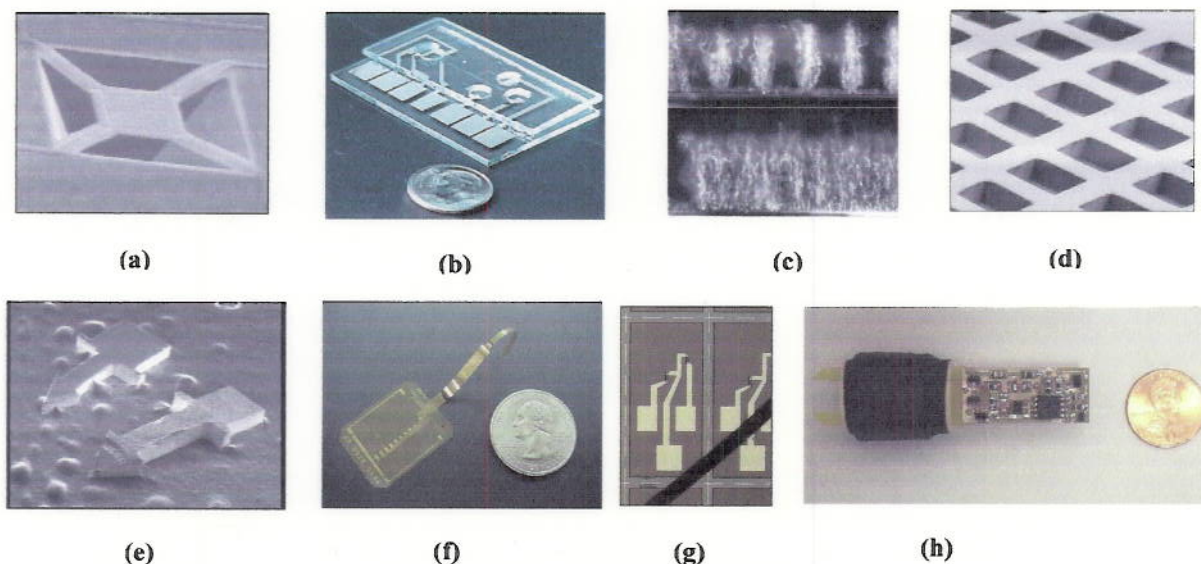


Fig. A1. Selected nano-structures and MEMS-based micro-devices developed by the UofL Group B Research Team over the past 2 years: (a) micro-hotplate for gas sensing applications, (b) lab-on-a-chip (LOC) device for chemical separation and analysis using on-chip electrochemical detection, (c) selectively grown carbon nano-tubes on patterned oxidized silicon, (d) high aspect ratio micro-well arrays formed in SU-8 for ORNL DNA hybridization research, (e) DRIE-ed silicon and micro-milled titanium micro-tacks (250um thick) for attachment of bio-devices to soft tissue, (f) polyimide micro-electrode array for retinal implantation (9 um thick), (g) subminiature biomedical pressure sensors compared to a human hair (80 um), and (h) hybrid RFID wireless telemetry device for remote temperature sensing.

B4. Educational Opportunities

The materials research funding generously provided by the DOE EPSCoR program has translated into numerous educational and scientific outreach opportunities for students and post-graduates in the state of Kentucky. The Group B component has directly funded 5 graduate students (1 female) and 1 senior

scientist over the last 2 years. Indirectly, the grant has affected an order of magnitude more individuals. Research developed as a part of this grant has been incorporated into 5 UofL courses in the areas of microfabrication, MEMS design, bioMEMS, nanotechnology and advanced microelectronic fabrication. These courses are offered annually, with the hands-on microfabrication course (ECE544) offered each semester. In total, well over 100 undergraduate and graduate students from various disciplines (EE, ME, ChE, CompEng, Chem, Physics, and Medicine) have been exposed to the benefits and potential of these new technologies. Other outreach programs initiated as a part of this grant have included: a) a valuable summer internship in the UofL MicroTechnology Cleanroom for a local freshman engineering student attending Johns Hopkins University, b) lectures to the junior and senior Physics classes of Trinity High School, a premier science and technology high school in Louisville, KY, c) presentations to over 1,000 high school students at the Intel International Science Fair competition, and d) cleanroom tours to several groups of African-American female high school students as a part of Career Day for Women. All of these programs will continue as an important part of the DOE renewal proposal.

B5. Proposed Research

Focus Area B contains 6 individual projects, all related to the applications of nanoscale materials for the design and development of microelectronic and MEMS-based devices and systems. The projects range from fundamental experimental studies of nano-scale molecules for microelectronic applications to the development of MEMS-based microsystems of use to DOE in the areas of environmental, industrial and biomedical sensing. The projects proposed in this research build upon our team's success during the first 2 years of DOE EPSCoR funding.

B5.1 Single Molecule Electronic Devices (B.Alphenaar and B. Hinds – project leaders)

Introduction: The goal of this study is to fabricate electronic, and spin-electronic devices based on individual, chemically engineered molecules. Molecular based electronics provide new functionality and an order-of-magnitude reduction in device size compared to the best possible efforts of silicon technology. This allows for ultra-high density circuits and extremely sensitive biological and chemical detectors. For spin-electronics, ferromagnetically contacted molecules can be used as a means to detect and manipulate single electron spins. This not only provides for high-density magnetic memory and sensing, but is also an essential component of recently proposed quantum computational schemes. [B1.1]

DOE Interest and Interaction: This project overlaps with a number of research focus areas of the Solid State Division at Oak Ridge National Laboratories. [B1.2] S. Pennycook and Z. Zhang are currently working on the synthesis of functional nano-building blocks, using nanocrystal compounds for molecular scale electronics and sensors. S. Kalinin and A. Baddorf are pursuing nano-electronic switches, transistors and devices for quantum computation. Meanwhile, J. Shen and J. Thompson are striving towards understanding magnetism in dimensionally confined systems and the control and exploitation of spin and spin-currents. Our proposed work would be of interest to any of one of these groups, and efforts will be made to establish direct interaction with ORNL.

Results to Date: Bruce Alphenaar provides expertise in the fabrication and measurement of molecular junctions. His important contribution in this area is the first observation of coherent electron spin transport through a carbon nanotube, reported in *Nature* in 1999. [B1.3] For the current project his group has already patterned sub-100 nm width ferromagnetic leads, and effort is now focused on creating 1-2 nm break junctions for molecular contacts. Bruce Hinds' chemistry background is well suited to synthesize a variety of target chelating molecules with discrete numbers of C-linking groups, and to use coordination compounds to bridge the break junction gap. He has an active research program in manipulation of carbon nanotubes, and recently developed a method to control the CNT diameter simply by the thickness of an exposed cross-section of a SiO₂ film [B1.4].

Plan of Action: We plan to fabricate single molecule transistor structures by bridging a 1-2 nm gap in a gold electrode with a single metal ion connected by a string of terpyridines ligands (see Fig. A2). [B1.4] The gold contact wire will be patterned on the surface of a SiO₂ / Si substrate so that the back silicon layer can act as a gate electrode. We will explore two techniques to form sub 10 nm gaps in the wire. Passing an increasingly large current through the wire will eventually form a gap due to electron migration of the gold. If the wire resistance is monitored during the electron migration process, the size of the gap can be controlled to nanometer resolution. [B1.5] A second possibility is to use a 1-2 nm diameter carbon nanotube suspended between two pillars as a shadow mask to form a nm wide break in the metal lines. Work is now underway to fabricate such a nanotube structure at University of Kentucky. To attach the molecules to the contacts, thiol terminated ligands will be drop-cast from solution onto an array of gold wires, and will self-assemble onto the gold surface. The resistance of a number of wires will be tested to find locations in which ligands have bridged the gap in the wire. Once located, we can electrically characterize the molecular devices. We expect for the ligands to act as simple tunnel barriers, so that the current will be controlled by the availability of electron states within the metal ion, modified by a large Coulomb-charging barrier. [B1.6] The energy states within the ion can be shifted with the gate bias, allowing for transistor action to occur. The device structure can also be used to determine the electron energy spectrum of the metal island.

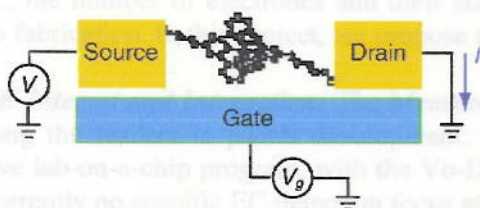


Fig. A2. Schematic drawing of our molecular device structure consisting of two tethered Tripyridine ligands coordinated to a single metal ion in a nm-scale gap between Au electrodes.

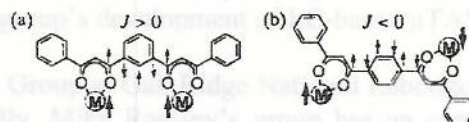


Fig. A3. Example of how the number of linking atoms in a ligand can be used to transfer spin information. (Matsushita et al., N. Mataga)

An important part of our work will be to determine possible spin-electronic applications of molecular devices. The gold leads can be replaced by 70% Au 30% Fe leads, which are ferromagnetic at room temperature. [B1.7] If the metal ion spin state is aligned parallel to the leads, the resistance will be lower than in the anti-parallel state. This state can be easily detected and act as a Q-bit for quantum computing applications. An exciting possibility is to control the spin state of the metal ion by changing the length of the ligand chains. [B1.8] Coupling can be altered from ferromagnetic to anti-ferromagnetic by changing the length of the ligand by one carbon atom. (Fig. A3) This in effect allows spin information to be transferred from the contacts to the ion.

B5.2 Self-contained μ TAS Devices with Electrochemical Detection (R. Baldwin - project leader)

Introduction: Within the past decade, the idea of constructing “micro total analysis systems” (μ TAS) incorporating a range of sample processing and analysis operations onto a single microfabricated chip has progressed from a research curiosity to a commercial product [B3.1, B3.2]. To date, the most common detection technique used in μ TAS systems has been laser-induced fluorescence (LIF). Although LIF has played a key role in successful μ TAS applications involving DNA analysis and gene sequencing [B3.3, B3.4], this detection method suffers from some drawbacks. Most important, LIF uses optical components – laser, monochromator, photomultiplier or photodiode array – that are external to the μ TAS and, in fact,

applications is carbon, and the adaptation of current fabrication techniques for patterning on-chip carbon electrodes will be a priority. Also, the fabrication of potentiometric ion-selective electrodes will be considered as well. Second, we will examine our cell design (see Figure A5b) and determine the effects of changes in electrode size, shape, etc. on device performance. It seems likely that such design details should play an important role in both potential control and signal/noise levels [B3.8-B3.10]. Third, we have as our ultimate goal the construction of complex CE/EC μ TAS devices containing electrode arrays capable of performing multiple determinations (e.g., several analytes in one sample). Success here will clearly be facilitated by our ability to access different electrode materials and to configure the electrodes optimally on the microchip. The vast majority of μ TAS applications to date have focused on biological and life sciences [B3.2]. While the importance of these areas (e.g., clinical diagnostics, immunoassays, and DNA analysis) is unquestionable and EC detection may well make meaningful contributions to them, μ TAS have largely bypassed applications involving “routine analysis” – e.g., pH, Cl^- , F^- , heavy metals, NH_3 and simple amines, etc. Such determinations are often well suited to EC detection (both amperometric and potentiometric), and there exists a large body of knowledge describing well behaved but macro-scale electrodes for these analytes [B3.11]. Adapting such electrodes to the μ TAS environment would have many applications in environmental monitoring, industrial process control, and remote sensing that are well matched to our fully portable lab-on-a-chip instrumentation. Accordingly, this project will focus specifically on the development of new CE/EC systems for such “simple” analytes.

B5.3 MEMS-based Multi-Species Fluid Analysis Device (K. Walsh – project leader)

Introduction: Basic MEMS fluidic sensors have been used to monitor the elevated temperatures generated by mixing acids and bases and similar energetic reactions. Zieren and Kohler have demonstrated such a device with two inlets, a mixing zone and down-stream thermopiles [B2.1]. Unfortunately, such methods do not discriminate between different species. This is both a benefit and liability. On one hand, a single sensor can be used in many applications; however, in an environment of mixed fluids the sensor can react to the combined concentration of all reactive compounds. Other liquid sensors have used methods such as mass absorption and, more recently, enzymatic based devices [B2.2].

The incorporation of biological molecules in sensors is a promising direction in MEMS devices. Biological molecules allow tailoring the sensor response to specific agents in a sample. Furthermore, arrayed sensors with unique biological molecules allow parallel testing of a single sample for an entire range of metrics. Of course, such a device is a very complex system of sensors and electronics. The University of Louisville is working toward producing such a device. The initial step will create a device with the capability to detect a single agent within a fluidic sample. Further development will expand the working principle to generate an array of sensors on a single chip, each discrete sensor coated with a unique enzyme such that a single sample will be tested for multiple constituents at the same time. Finally, the device will be integrated into a microfluidic system allowing the testing of many samples in succession.

DOE Interest and Interaction: The University of Louisville has been working with Oak Ridge National Labs (ORNL) on this project. In particular, Dr. Mitch Doktycz has acted as our contact providing his expertise in the biological foundations of the device operation. As a member of the Life Sciences Division, he has contributed to the development of ORNL’s biomedical engineering program to provide an integrating focus for several research efforts, such as medical telesensors, biosensors, medical diagnostics, biological systems modeling, and analytical technologies.

Results to Date: Our work has begun by capitalizing on an enzyme immobilization technique investigated by ORNL [B2.4]. We are jointly developing a set of chips (Fig. A4) to test the sensitivity of micro-calorimeters to basic enzyme/analyte reactions in a static fluid environment. These incorporate a platinum thermal coefficient of resistance (TCR) sensor on a bulk micromachined membrane of low-

stress PECVD silicon nitride and silicon dioxide. Each membrane is 1.2mm x 1.2mm which allows sufficient area for the platinum sensor and still provides thermal isolation from the bulk of the chip. To this surface, a coating of glucose oxidase (GOD) is fixed with poly-L-lysine as outlined in the ORNL method. Therefore, the introduction of a glucose solution to the sensor produces an exothermic reaction that is translated into a voltage signal. We are currently characterizing the glucose/GOD reaction and evaluating the best method of obtaining a consistent signal. The experiments are being run across a range of temperatures to determine the optimal response time and reaction temperature.

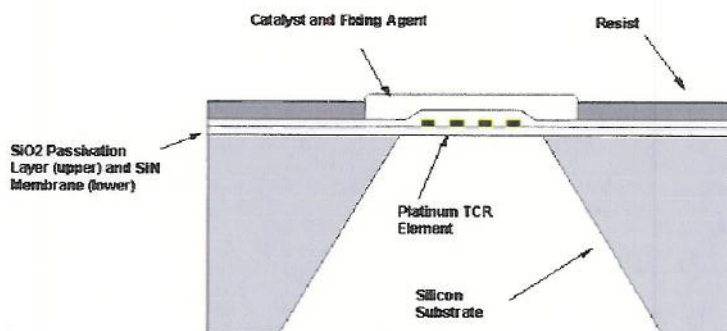


Fig. A4. Cross section of the micro-calorimeter device designed in collaboration with ORNL

Plan of Action: In the pursuit of a sensor capable of multiple simultaneous analysis on a single sample, we have identified several areas of development: individual sensor size and response (covered in the previous section), integrating an array of sensors on an easy to use device, and incorporating microfluidics to achieve a working prototype of a commercial device. Once the single species sensor is functioning well, other enzyme/analyte pairs will be investigated such as lactate and lactate oxidase and incorporated into an array of sensors on a single chip. Each element of the sensor matrix will be created in the same manner as before but this stage of development will benefit from technologies such as our deep reactive ion etcher that creates nearly vertical walls on bulk micro-machined features significantly reducing the amount of real estate each sensor requires and thereby increasing the density of the sensor array. By tailoring the list of enzymes applied to the device, it can be customized to fit a range of applications. After establishing a functioning sensor array, microfluidics will then be integrated on-chip to cycle through individual samples and increase throughput. Computational flow dynamics using the software MEMCAD will be utilized to optimize the design and operation of the microfluidic flow structures. This final prototype will be an excellent candidate for a commercial device with applications in the biomedical field such as blood analysis or cell composition determination.

B5.4 Bioelectronic MEMS Detectors for Chemical and Biological Warfare Agents (R. Keynton - project leader)

Introduction: Recent terrorist attacks on the US have spawned new DOE-sponsored homeland security initiatives, such as, real-time detection systems for chemical and biological warfare agents, to ensure the protection of, not only military personnel, but also the civilian population [B.4.1]. In response to these initiatives, we developed a novel concept to fabricate bioelectronic devices that utilize an artificial cell wall with associated membrane transport enzymes to produce a simplified model of the neuromuscular junction for the broad-spectrum detection of nerve agents. Biomolecules have been used in the development of microsensors for biochemical detection, such as glucose, urea, etc. [B.4.2-B4.6]; however, limited research has been conducted in bioelectronics and the incorporation of biomolecules as a transduction method for nerve agent detectors [B.4.16]. The proposed detection scheme is based on the functional reconstitution of enzymes in an artificial cell wall (a phospholipid bilayer) specifically arranged to produce electrically separate aqueous cells, which are supported on a hydrophobic

microfabricated lattice. For this application, the enzyme, acetylcholinesterase (AChE), and a ligand-gated channel, acetylcholine receptor (AChR), will be reconstituted from the neuromuscular junction into the lipid bilayer [B.4.17, B.4.18]. The mechanism of operation of the device will mimic the biological situation where AChR is opened when the neurotransmitter acetylcholine (ACh) ligands to it, subsequently, the ACh is gradually reduced by AChE (hydrolyzing it to choline) and allowing the AChR to close. Initially, this project will focus on detecting post synaptic nerve and chemical agents, such as Sarin(GB), Tabun(GA), Soman(GD), and VX, since exposure blocks the action of AChE causing the membrane to remain conductive indefinitely.

DOE Interest and Interaction: This innovative approach could find applications in environmental sensing, and drug and general biochemical research, etc., which are of interest to DOE laboratories. Specifically, Dr. Doktycz's (ORNL) and Dr. Hughes' (SNL) groups are independently investigating the use of lipid bilayers for biological and chemical warfare detection; however, their manufacturing techniques involve using self-assemble monolayer and sol-gel film techniques, which differ from the proposed fabrication technique. Other researchers at Pacific Northwest and Sandia (SNL) National Laboratories have also developed microsensors for Sarin (post-synaptic nerve agent) detection [B.4.19].

Results to Date: This project represents a new research area for the team that spawned from cross-disciplinary interactions initiated from the local infrastructure and expertise in MEMS fabrication, nanoscale metrology, and microfluidics gained from the current DOE support.

Plan of Action: Initially, prototypes will be produced with apertures formed in surface modified low stress silicon nitride (Si_3N_4) films to investigate the influence of perforation geometry (circular vs. rectangular holes), array density and pitch, and diaphragm thickness and surface modification techniques on pure lipid bilayer stability. Fabrication will consist of: 1) thermally oxidizing a (100) Si double-sided polished wafer; 2) PECVD a low stress Si_3N_4 layer (1-5 μm) on one side of the wafer; 3) electrode sputter deposition and patterning; 4) depositing a hydrophobic layer using either spin-on Teflon[®], vapor deposited siloxanes [B.4.7], plasma-deposited Teflon[®] or spin-coated polyimide and patterning via plasma etching techniques; 5) plasma etching the apertures into the nitride layer; and, 6) patterning a window in the oxide and bulk anisotropic etching to release the Si_3N_4 .

The lipid bilayer will be developed using the liposome-based reconstitution technique [B.4.8] since it offers many of the advantages of the Langmuir-Blodgett bilayer technique without requiring a film balance and lends itself to automation. This technique allows proteins to be reconstituted asymmetrically and increases surface tension (and bilayer stability) by increasing the diameter of the liposomes in solution [B.4.8-9]. Experiments indicate that a minimum lipid monolayer lateral pressure of 25-30 dyne/cm² is required before a stable bilayer can be formed [B.4.8]. The reconstitution technique proposed does not allow independent control of the surface pressure; however, using monolayers produced from liposome suspensions enables empirical tuning of the surface pressure by adjusting liposome diameter as well as bilayer composition.

Second-generation prototypes will be developed to demonstrate asymmetric reconstitution of AChE and AChR by integrating the bilayer support with a perfusion system and chamber into a single planar device. The device will consist of three layers (from bottom to top): 1) a soda-lime glass plate ($t \sim 2\text{-mm}$) for conductivity sensor fabrication and sealing of the bottom perfusion ports, 2) a bulk micromachined silicon wafer ((100); $t \sim 0.5\text{ mm}$) to form a thin tilted membrane for bilayer support and microfluidic channels (both front and back), and 3) a second soda-lime glass layer ($t \sim 0.1\text{-}0.2\text{ mm}$) to seal the bilayer support chamber and top perfusion ports. Subsequently, the remaining design elements to be introduced to produce a functional nerve agent/toxin sensor include: 1) valve designs with diaphragms based on Si [B.4.10], PDMS (polydimethylsiloxane) [B.4.11] or polyimide [B.4.12]; 2) actuation produced via thermopneumatics [B.4.13], shape memory materials [B.4.12 & 14], or electro-magnetics [B.4.15]; and,

3) pumps produced by electro-kinetics, electro-mechanical systems or compressed gas. Control logic will be used to actuate the valves and pumps, which should require little more than a PLC (Programmable Logic Controller). To determine detection of a nerve agent, small amounts of ACh will be introduced on one side of the lipid bilayer through microfabricated perfusion ports. In the event an agent is not present, the ACh will be hydrolyzed to choline and the membrane resistivity will increase. In the event an agent has blocked the AChE, the membrane resistivity will remain low. After polling, the choline will be removed via the perfusion ports assuming a negative result. In the event of a positive result, the bilayer will be purged from the device and automatically reconstituted. Enzymes and lipid bilayers will be characterized primarily by observing electrical properties such as capacitance and resistance per unit area.

B5.5 Ultra- High-Precision Micromechanical Machining of Ceramic Materials (R. Keynton - project leader)

Introduction: Development of high temperature MEMS devices – particularly for strain, temperature and pressure measurement – will provide a significant benefit for new advanced energy systems. MEMS sensors embedded within advanced combustion systems, turbine engines or high-temperature fuel cells can provide detailed monitoring and precise control of these systems, producing improved efficiency and reduced emissions. The application of microfabrication techniques to mechanical systems has led to a dizzying array of miniature sensors, actuators, pumps, engines and other devices [B.5.1]. The range of applications seems limited only by the imagination of the designers. *Yet there are real limits – based on materials as well as applications involving high temperatures and aggressive chemical environments.* Thus, we propose to investigate a new MEMS fabrication approach that offers the potential for forming high aspect ratio structures with excellent geometric accuracy using a variety of oxide and nitride ceramics for creating high temperature MEMS devices for advanced energy systems. This new fabrication method consists of ultra- high-precision micromechanical machining in combination with atomic layer chemical vapor deposition (ALCVD) and offers significant advantages over traditional, silicon-based methods since micromilling *can be used with a wide variety of materials and can easily produce high aspect ratio structures* and ALCVD *is completely conformal and produces thin films with incredible thickness accuracy on complex, high aspect ratio structured surfaces.*

DOE Interest and Interaction: The proposed high temperature MEMS devices will be fabricated in collaboration with Dr. Tom Starr, Department of Chemical Engineering at the University of Louisville, and Dr. Theodore M. Besmann, Head of Surface Processing and Mechanics Group, Metals and Ceramics Division at ORNL, both of whom have expertise in ALCVD.

Results to Date: A custom-made, ultra- high-precision micro milling and drilling machine was purchased from Dover Instruments, Inc. with funds acquired from DOE Phase I funding. The machine was received in April 2002 and installed by June 2002. The machine has been utilized in several studies including: development of a fiber optic-based microphone, retinal prosthesis microtacks and an explosive detector (Figure A6). The machining processes for several materials such as glass, titanium, aluminum and stainless steel, have been characterized to optimize surface roughness, structure integrity, machining time, and tool wear by varying spindle speed, depth of cut, feed rate and lubrication fluid. The proposed project is a new area of research that spawned from the local infrastructure and expertise acquired through the current DOE support.

Plan of Action: High aspect ratio 3-D structures will be directly machined in alumina and glass using the custom-made, ultra-precise, mechanical machining system, which produces microscale feature sizes with high aspect ratios and has nanometer machining resolution and process repeatability. The machining processes will be characterized and optimized for feed rate, depth of cut per pass, spindle speed, tool design, tool performance and tool coating as well as lubricating fluids (water-soluble cutting oils vs. water-based diamond slurries). In this project, custom-made 35 μm end-mills (Figure A6) will be

machined at SNL through their micro tool collaborative program using FIB milling. For this study, the end-mills will be coated with diamond or diamond-like films using the CVD processing systems at U of L to enhance tool wear resistance and machining performance, followed by FIB milling to "resharpen" the cutting edges.

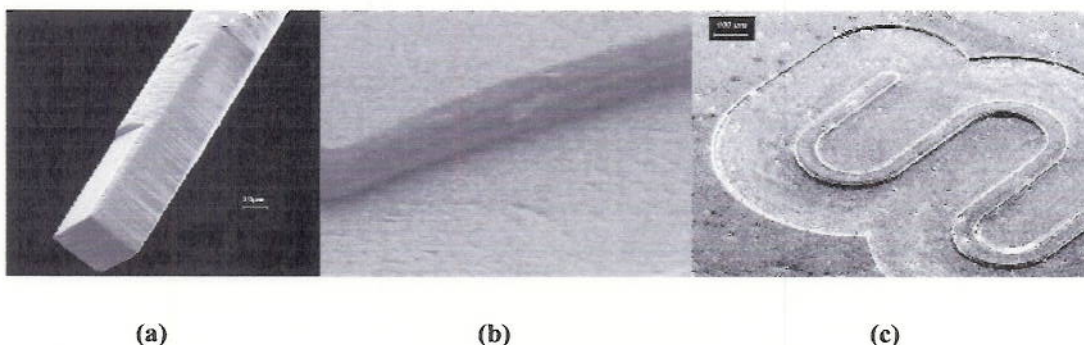


Fig. A6. Images of: (a) high speed tool steel 35-micron end-mill, (b) sidewall of a micromilled channel on the tip of an optical fiber (3500X), and (c) serpentine pattern micromilled in glass for ceramic strain gage.

ALCVD is a variation of the standard CVD process and involves two separate reactants delivered to the surface as discrete pulses [B.5.2, B4.3]. One pulse of a metal-containing precursor leaves a chemisorbed monolayer on the material surface and a second pulse of a reactant species converts this to a monatomic layer of solid, deposited film. The process is self-limiting, completely conformal and produces thin films with incredible thickness accuracy. Each two-step cycle of ALCVD produces a monolayer of deposit, i.e. roughly 0.1-0.4 nm of solid oxide, thus a 1.0- μ m film requires 10,000 to 2500 cycles, respectively. Experimental investigation of ALCVD in this study will use an existing CVD reactor at ORNL [B.5.6]. Basic deposition parameters will be controlled independently by variation of gas velocity, pressure, reactant concentration, and nozzle and substrate temperatures. Modification of this reactor for ALCVD will require replacement of the existing steady-state, single precursor reactant supply system with a pulsed, cycling precursor and reactant supply system. Our design will provide for separate precursor/reactant species, controlled flow of carrier gas and a temperature-controlled volatilization region.

B5.6 Telemetry Development for a Retinal Prosthesis (J. Naber – project leader)

Introduction: The leading cause of legal blindness in the industrialized world is age-related macular degeneration (ARMD) and the second leading cause is retinitis pigmentosa (RP). Neither disease can be treated to restore lost function. The number of patients affected by these diseases (700,000 Americans each year develop ARMD and 1.6 million people worldwide have RP) makes a compelling case to pursue a solution [B6.1].

The concept of a retinal prosthesis was motivated by the cochlear implant, which has restored useful hearing to a number of deaf patients. ARMD is caused by a cell mutation that leads to the loss of the majority of photoreceptors. However, the inner retina that is connected to the brain via the optic nerve is relatively spared. Theoretically, a prosthesis could be made to bypass the lost photoreceptors by directly stimulating surviving retinal neurons either sub-retinally or epi-retinally. There are four primary groups throughout the world pursuing various types of retinal prostheses to improve the quality of life for people stricken with these diseases [B6.2-B6.5].

DOE Interest and Interaction: DOE has funded a \$9 million, three-year grant from the Office of Biological and Environmental Research to create an epi-retinal prosthesis using a 33 x 33 electrode array

[B6.2, B6.6]. The lead lab, Oak Ridge National Laboratory (ORNL), is managing the multi-laboratory effort as well as testing the various components developed by the other DOE labs. Our group has made multiple trips to visit and discuss collaborative projects with the Wireless Design group at ORNL and we will plan on interfacing with them on this project as well.

Results to Date: Radio Frequency Identification (RFID) [B6.7] telemetry gives the Multi-Electrode Array (MEA) the ability to send data through the eye without wires or batteries. Wires are impractical due to infection concerns and batteries are too large and have a finite lifetime. Therefore, this device will require wireless transmission of the electrode data from the image sensor outside the eye to the MEA chip inside the eye without wires or batteries.

Most wireless devices operate using batteries for their power source. RFID technology uses the magnetic field coupling between two closely spaced coils to induce a voltage from one coil to another, similar to how a transformer operates. However, RFID uses a capacitor on the secondary coil to store a voltage that powers the electronics without requiring batteries and uses a technique called backscatter modulation to send on-chip data back to the outside world. RFID technology consists of two primary components: a reader and a transponder.

The reader or primary coil supplies power to the implant circuit via an inductive link between the two coils and receives data from the implant by detecting the varying electrical load produced by the implant circuit. These systems operate at the FCC approved ISM frequencies of 125kHz or 13.5MHz with the most common application being inventory and identification. In these applications, an identification string is transmitted across the inductive link. By adding circuitry to the RFID circuit, a current source array can be integrated and digitally encoded data transferred across the inductive link from the reader to the secondary coil to active a particular current source.

Plan of Action: Some of the novel concepts our group will be pursuing in the telemetry research are using two coils for the design. One optimized for power transfer at 125 KHz and the second optimized for data transfer at 13.56 MHz. All other research groups have had to make the tradeoff between data rate vs current by using a single coil design.

Our group will also be evaluating options on the critical design and placement of the secondary coil, which generates the current for the MEA and control electronics. The voltage developed on the coil is determined by the: frequency (f), number of coil turns (N), quality factor (Q), coil area or size (S) and the magnetic field (B) is given by the following equation [B6.8]:

$$V = f \times N \times Q \times S \times B$$

The primary coil diameter on the glasses will be fixed with a 2" to 3" coil diameter and the current through the primary coil will be limited by the Federal Communication Commission (FCC) regulations for electromagnetic exposure limits [B6.9]. An E-field and H-field meter will be used to validate the maximum power into reader coil is within the FCC, Institute of Electrical and Electronics Engineers (IEEE) and international guidelines [B6.10]. The thickness of the coil will be evaluated as will the number of turns. Increasing the number of turns increases the flux density (resulting in more induced voltage on the tag) at the expense of more wire. Increasing the coil thickness will reduce the series resistance or loss (Q) in the coil at the expense of increased wire area.

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IV. MAJOR FACILITIES, EQUIPMENT and RESOURCES

Microfabrication Cleanroom Facilities: (UofL) The Lutz Microtechnology Cleanroom is a state-of-the-art 1500 sq. ft. class 100 facility containing several processing bays, 2 fume hoods, 2 vertical laminar flow wet processing stations, and a recirculating 18.3 MegOhm DI water system. (UK) The Center for Micro-Magnetic and Electronic Devices has recently been established and contains a class 100 photolithography bay.

Lithography: (UofL) Heidelberg Laser Writer Pattern Generator, NPGS Electron Beam Writing System, Karl Suss Front/backside Alignment/Exposure System, ABM Backside Mask Aligner and Exposure System, 2 Quintel Contact Mask Aligners (UK) Raith 50 Electron Beam Writing System, Karl Suss MJB 3 HP Infrared Mask Aligner.

Deposition and Thermal Processing: (UofL) Technics RF/DC Sputterer, STS PECVD System, Rapid Thermal Processing/Anneal (RTP/RTA) System, 2 Thermal Oxidation Systems, 2 Thermal Diffusion Systems, Denton Thermal Evaporator, DC Sputter/Coater (UK) AJA International 5 Gun Sputtering System, Edwards High Vacuum Coater, TEK-VAC Plasma CVD System, TORR International E-Beam Evaporator, Doping and Annealing Furnaces.

Etching: (UofL) STS Deep Reactive Ion Etcher (DRIE), March Instruments RIE System, SemiGroup RIE System, 4 Anisotropic Etching Systems, 2 VLF Wet Processing Stations (UK) Technics Ion Milling System, Electrotech RIE, Laminar Wet Processing Stations, PCT Megasonics Anisotropic Etch Tank.

Surface Characterization: (UofL) Tencor Profilometer, Filmetrics Spectroscopic Ellipsometer, Park Scientific M5 and CP Atomic Force Microscopes, WYKO NT-2000 white-light scanning interferometric microscope, 3 High Power Optical Microscopes with Digital Cameras (UK) Tencor Surface Profiler, Gaertner Ellipsometer, DI Instruments IIIa Multimode Scanning Probe Microscope, Olympus Research Microscope.

Micromachining, Bonding and Packaging: (UofL) Dover Ultra-High-Precision Micromilling / Drilling System, Karl Suss Wafer-level Bonding System, Custom Electrostatic Bonding System, Logitec Wafer-level Polishing System, K&S Wedge and Ball Wirebonders, Disco Diamond Dicing Saw (UK) Micro Automation Dicing Saw, Westbond Wirebonder.

Electron Microscopy: (UofL) LEO 1430 and JEOL 5310 thermal emission SEMs (UK) Hitachi 3200S Variable-Pressure SEM, Hitachi S900 Field Emission SEM, JEOL 2000FX TEM, JEOL 2010F Field-Emission TEM.

Flow and Pressure Sensing: (UofL) 8 channel/20 MHz pulse ultrasonic Doppler system, Transonic flowmeter and flow probes, real-time spectrum analyzer data acquisition system; a multi-channel variable speed roller pump; a 5 MHz MicroMAX 1385x1060 12-bit digital CCD camera, a 10W Argon-Ion laser; 2 Fourier lenses; 1 collimating lens; 2 knife edges, and a microfluidic flow visualization system that includes a Zeiss light microscope with a 3-D positioning controller.

Electrical Characterization: (UofL) 4-Point Probe Conductivity System, Probe Station, HP 8410 Network Analyzer, HP 435 power meters, HP high frequency sweepers, spectrum analyzers, Two RF Screen rooms, Signal Generators 0 to 3.2 GHz, Microwave Oscillators to 12 GHz, Agilent mixed signal oscilloscopes, Network Analyzers to 3GHz, Communication Analyzer to 1GHz, Time Domain Reflectometer, Spectrum Analyzers to 3.0 GHz, Semiconductor parameter analyzer (UK) HP4155B semiconductor parameter analyzer, HP E5250A low leakage switch main frame, HP8160A programmable pulse generator, Keithley 595 quasistatic CV meter, Keithley 590 CV analyzer, and Alessi REL-2000 probe station, 4-point probe resistivity system (Signatone).

Low Temperature Characterization: (UofL) Janis variable temperature cryostat 1.5-300K with 9T magnet, Leiden Cryogenics 500 W dilution refrigerator with 9T magnet, Janis Research optical flow cryostat with temperature control, Desert Cryogenics variable temperature probe station (UK) Janis Industry low temperature (4K) magnetic field (2T) transport (fA resolution) measurement station.

Optical Characterization: (UofL) Spectra-Physics fs pulsed OPA laser system, Roper Scientific CCD imaging spectrometer, Walker Scientific 1T electromagnet with optical access, Nanonics Near Field Scanning Optical Microscope, Surelite I YAG laser.

Chemical Analysis: (UofL) Two benchtop capillary electrophoresis units (home-built, electrochemical detection), two Bioanalytical Systems Model CV-50W electrochemistry workstations, a Pine Instruments Model RDE4 dual-electrode potentiostat with rotating electrode capabilities, and a flow injection system with electrochemical detection. **(UK)** ATI Solvent glove box with spin coating and electrochemical station, Schlink line and synthetic chemistry fume hoods, Standard synthetic chemical laboratory (with access to university analytical services), 3-zone oxidation and annealing furnace.

Computer Facilities: (UofL) A Beowulf system (26-athlon-processor-Linux clusters) and a SGI-Origin 2000 system (16 processors), access to the Risc-based IBM supercomputer (112 processors), MEMCAD software installed on two dual-processor machines (Pentium III and a Xeon) each with 1.0 GB RAM.

V. CURRENT AND PENDING SUPPORT

Current Support:

Joint Grants of Members from both Projects A and B:

1. DOE – EPSCoR: *"Integrated Materials Architectures: From Nanoscale Studies to Microdevice Development"*; PIs: K. M. Walsh (PI), R. S. Keynton, R. P. Baldwin, J. F. Naber, C.S. Jayanthi, S. Liu, S.Y. Wu, B. W. Alphenaar, Craig Grimes, Elizabeth Dickey, Susan Sinnott, and Andrew Mason; \$952,452; 9/00 – 8/03. (Dr. Walsh is PI of the UofL MEMS effort, Dr. Jayanthi is PI of the UofL Physics/ Nanoscience effort and Dr. Grimes is PI of the UK MEMS effort.)
2. NSF-ONR: *"Carbon Nanotube based Spin Electronic Devices"*; PIs: B. Alphenaar (PI), C. Jayanthi, and Shiyu Wu, \$450,000, 10/1/02 – 9/30/05.

Project A:

1. NSF-DMR-0112824: *"Large-Scale Quantum Mechanical Molecular Dynamics Simulations: Challenges, New Directions, and Applications to Carbon-Based Nanostructures"*; PIs: C.S. Jayanthi (PI) and S.Y. Wu; \$456,000; 8/31/01-07/31/04.
2. NSF-CAREER: *"Fundamental Reliability Physics of MOS Devices Based on Deuterium Isotope Effects"*; PI: Zhi-Chen; \$374,877; 03/01 – 03/06.

Project B:

1. NSF – EPSCoR: *"Biomedical Nano- and Micro-Electro-Mechanical Systems"*; PIs: R. Keynton (PI), K. Walsh, B. Alphenaar, K. Kang, J. Naber, G. Pantalos, E. Wang; \$2,490,056; 3/02 – 2/05.
2. NSF – MRI: *"Implementation of Deep Reactive Ion Etching Technology for the Advancement of Micro/ Nanotechnology Research at the University of Louisville"*; PIs: K. M. Walsh (PI), R. S. Keynton, R. P. Baldwin, J. F. Naber, R. W. Cohn, T. Starr, E. Brehob, H. Cox, and M. Sunkara; \$333,000, 9/00 – 8/01.
3. NSF – XYZ-on-a-Chip: *"An Integrated Monolithic Capillary Electrophoresis System with Electrochemical Detection"*; PIs: R. Baldwin (PI), K. Walsh, R. Keynton and J. Naber; \$520,000; 10/99 – 12/02.
4. DoD – EPSCoR: *"Large Area Nanolithographic Fabrication of Photonic Components"*; PIs: R. W. Cohn (PI), K. M. Walsh and M. Sunkara; \$429,950; 4/00 – 3/03.
5. NSF – XYZ-on-a-Chip subcontract through University of Missouri-Columbia: *"Cellular Electrophysiology on a Chip"*; PI: R. Baldwin; \$98,331; 10/00 – 9/03.
6. NSF: *"A Real Time Monitoring System for Spinal Fusion Surgery"*; PIs: W. P. Hnat (PI), K. M. Walsh, J. F. Naber and M. J. Voor; \$348,948; 5/01 – 4/04.
7. Kentucky Science and Technology Corporation (KSTC): *"Glaucoma Sensor Development"*; PIs: J. Naber (PI), K. Walsh, R. Keynton, and H. Kaplan; \$225,000; 10/02 – 9/05.
8. Veterans Administration (VA) subcontract through Harvard/Massachusetts Eye and Ear Infirmary: *"Fabrication of an Artificial Retinal Implant"*; PIs: H. Kaplan (PI), K. M. Walsh, R. S. Keynton and J. F. Naber; \$94,000; 9/02 – 9/03.
9. Naval Research Laboratory (NRL): *"Design and Fabrication of MEMS-based Chemical Sensing Platforms using Flow-through Micro-hotplate Technology"*; PIs: K. M. Walsh (PI), M. Crain and R. Keynton; \$110,000; 10/01– 4/03.
10. Southwest Research Institute (SwRI): *"Ultra-small Microphone"*; PIs: K. M. Walsh (PI), M. Crain and R. Cohn; \$94,682; 10/01 – 4/03.
11. SwRI: *"MEMS-based Thermal Microphone"*; PIs: K. M. Walsh (PI) and M. Crain; \$49,916; 7/02 – 8/03.
12. DoD – EPSCoR: *"Large Area Nanolithographic Fabrication of Photonic Components"*; PIs: R. Cohn (PI), K. Walsh, and M. Sunkara; \$429,950; 4/00 – 3/03.
13. NASA through Western Kentucky University: *"Nanofabrication of photonic crystals, nanotube spin electronics and nano electro-mechanical structures"*; PIs: R.W. Cohn (PI) and B.W. Alphenaar; \$510,000; 8/01-7/04.

14. NSF – ECS-MRI: *"Acquisition of a Virtual Presence Surface Profiling Microscope for Nanomanipulation and Nanoassembly"*; PIs: R. Cohn (PI), B. Alphenaar, M. Sunkara, and F. Zamborini; \$153,553; 05/02 – 04/05.

Pending Support:

Joint Grants of Members from both Projects A and B:

1. DOE – EPSCoR: *"Integrated Materials Architectures: From Nanoscale Studies to Micro/Nanodevice Development"*; PIs: K. M. Walsh (PI), R. S. Keynton, B. W. Alphenaar, R. P. Baldwin, J. F. Naber, C.S. Jayanthi, S.Y. Wu, G. Sumanasekera, A. Lowen, N. Miller, M. Yu, L. Liu, Z. Chen, and B. Hinds; \$3,150,000; 9/03 – 8/06. (Dr. Walsh is PI of the UofL MEMS effort and Dr. Jayanthi is PI of the UofL Physics/Nanoscience effort.)
2. DOE: *"Theoretical and Experimental Studies of Carbon Nanotubes, Carbon Nano-rings and Silicon Nanowires"*; PIs: Shi-Yu Wu (PI), C.S. Jayanthi, B.W. Alphenaar, and Jie Liu; \$1,354,683; 8/02-7/06.

Project A:

1. DoD – EPSCoR: *"Fabrication of Carbon Nanotube-Based Chemical Sensors and High-Speed Transistors"*; PI: Z. Chen; \$524,846; 06/03 – 05/06.
2. NSF: *"Advanced Lithography Based on Carbon Nanotubes: Sub-10 nm Patterning"*; PI: Z. Chen; \$313,660; 07/03 – 06/06.
3. NSF – NIRT: *"Carbon-Based Quasi-One-Dimensional Nanostructures: From Fundamental Science to Device Applications"*; PIs: S.Y. Wu (PI), C.S. Jayanthi, G. Sumanasekera, and Z. Chen; \$ 1,216,768; 07/03 – 06/07.

Project B:

1. NASA SBIR Phase I subcontract from SHOT, Inc.: *"Crystallization Micro Monitor"*; PIs: R. Keynton (PI) and K. Walsh; \$11,000; 3/03 – 9/03.
2. NIH – NEI SBIR: *"Real-Time Monitoring System for Measuring Intra-Ocular Pressure on Glaucoma Patients"*; PIs: J. Naber (PI), H. Kaplan, R. Keynton and K. Walsh; \$500,000; 2/03 – 1/05.
3. NASA: *"Shared Functional Genomics between Space-Flight and Aging"*; PIs: E. Wang (PI), B. Alphenaar, K. Falkner, T. Geoghegan, R. Keynton, C. Klinge, W. McGregor, R. Prough, and K. Walsh; \$1,499,924; 9/02 – 8/03.
4. DOE – EPSCoR: *"Diamond Based Electronic Devices"*; PIs: B.W. Alphenaar (PI), J.A. Carlisle and J. Gerbi (Argonne National Labs); \$450,497; 01/03 – 12/05.
5. DOE: *"Atomic Layer Chemical Vapor Deposition for Ceramic MEMS"*; PIs: T. Starr (PI), R. Keynton, and T. Besmann; \$623,521; 12/02 – 10/05.
6. NIH – NHLBI: *"A Fast, Multi-Blood Factor Deficiency Diagnostic System"*; PIs: K. Kang (PI) and R. Keynton; \$300,000; 6/03 – 5/06.

VI. BIOGRAPHICAL INFORMATION

KEVIN M. WALSH

*Director of the Lutz MicroTechnology Cleanroom,
Associate Professor of Electrical and Computer Engineering
University of Louisville, walsh@louisville.edu*

EDUCATION

Ph.D.	EE (Microelectronics)	University of Cincinnati	Aug 92
M. Eng.	Electrical Engineering	University of Louisville	Dec 85
BSEE	Electrical Engineering	University of Louisville	May 78

PROFESSIONAL EXPERIENCE

1996-present	Associate Professor, Electrical and Computer Engineering, University of Louisville
1997-present	Director, Lutz MicroTechnology Cleanroom, University of Louisville
1993-1996	Assistant Professor, Electrical and Computer Engineering, University of Louisville
1986-1993	Instructor, Electrical and Computer Engineering, University of Louisville
1986-1991	Research Fellow, ECECS Department, University of Cincinnati
1980-1986	Instructor, Engineering Math and Computer Science, University of Louisville
1976-1977	Applications Engineer, General Electric Appliance Park, Louisville, KY

RESEARCH INTERESTS

Microelectromechanical devices (MEMS), sensors and transducers, actuators, bulk and surface micromachining, anisotropic etching, microelectronic fabrication, electrostatic bonding, electrochemical etching, silicon-silicon bonding, piezoresistive effects in silicon, microaccelerometers, packaging, finite element modeling and analysis, device and process simulation, device physics, signal conditioning, temperature compensation, microprocessor applications, and VLSI design.

RELEVANT PUBLICATIONS

1. R. P. Baldwin, T. J. Roussel, M. M. Crain, V. Bathlagunda, D. J. Jackson, J. Gullapalli, J. A. Conklin, R. Pai, J. F. Naber, K. M. Walsh, and R. S. Keynton, "Fully Integrated On-Chip Electrochemical Detection for Capillary Electrophoresis in a Microfabricated Device", *Analytical Chemistry*, Vol. 74, No. 15, August 2002.
2. K. M. Walsh, R. P. Baldwin, T. J. Roussel, M. M. Crain, D. J. Jackson, J. F. Naber, and R. S. Keynton, "Integrated Electrochemical Detection for Lab on a Chip Analytical Microsystems", *WatchIT.com*, Jan., 2002.
3. S. Sharma, M. K. Sunkara, M. M. Crain, S. F. Lyuksyutov, S. A. Harfenist, K. M. Walsh and R. W. Cohn, "Selective Plasma Nitridation and Contrast Reversed Etching of Silicon", *J. Vacuum Science and Technology B*, Vol. 19, No. 5, pp. 1743-1746, Sept/Oct 2001.
4. S. C. Eaton, M. K. Sunkara, M. Ueno, K. M. Walsh, "Modeling the Effects of Oxygen on Vapor Phase Diamond Deposition inside Micro-trenches", *Diamond and Related Materials*, Elsevier Press, Vol. 10, pp. 2212-2219, 2001.
5. W. K. Pitts, K. M. Walsh, M. D. Martin and M. M. Crain "Effects of Well Diameter upon MicroWell Detector Performance", *IEEE Transaction on Nuclear Science*, Vol. 47, No. 3, pgs. 918-922, June 2000.
6. R. W. Cohn, S. F. Lyuksyutov, K. M. Walsh, and M. M. Crain, "Nanolithography Considerations for Multi-passband Grating Filters," *Optical Review*, Vol. 6, No. 4, pgs. 345-354, July/August, 1999.
7. J. B. Hutchins, W. K. Pitts, K. M. Walsh, M. D. Martin, S. Belolipetsky, H. L. Cox, "A Low-Cost High Performance Cleanroom Enclosure", *IEEE Transactions on Education*, Vol. 42, No. 2, pgs. 144-146, May, 1999.
8. K. M. Walsh, T. R. Hanley, W. K. Pitts, M. Crain, J. Cole, D. Hensel, J. Hernandez, and C. Foreman, "Development of a New Microfabrication/MEMS Course at the University of Louisville", *Proceedings of the 1999 IEEE University Government Industry Microelectronics Symposium*, Minneapolis, MN, pgs. 26-32, June 20-23, 1999.
9. K. M. Walsh, T. R. Hanley, W. K. Pitts, D. Hensel, J. Hernandez, M. Crain, and J. Cole, "Microfabrication Activities at the University of Louisville", *Proceedings of the 1997 IEEE*

University Government Industry Microelectronics Symposium, pp. 26-32, Rochester, NY, July 20-23, 1997.

10. W. K. Pitts, M. D. Martin, S. Belolipetsky, M. Crain, J. B. Hutchins, S. Matos, J. H. Simrall and K. M. Walsh, "Development of Laser Micromachined MicroWell Detectors", *Proceedings of the IEEE Nuclear Science Symposium*, Seattle, WA, Oct., 1999.
11. W. K. Pitts, K. M. Walsh, and K. Solberg, "Optical Imaging System Utilizing a Charge Amplification Device", Patent Number 5,602,397, Feb. 11, 1997.
12. W. K. Pitts, K. M. Walsh, and K. Solberg, "Radiation Detector Based on Charge Amplification in a Gaseous Medium", Patent Number 5,614,722, March 25, 1997.

AWARDS AND HONORS

Honored Member of *America's Registry of Outstanding Professionals*, 2002-2003

UofL Athletic Hall of Fame, 2001

Invited Speaker, *Microfluidics for Lab-on-a-Chip (LOC) Technology Seminar*, ASME, Sept. 9-11, Washington DC, 2001

Trinity High School Hall of Fame (one of only 39 recipients in Trinity History, presented in recognition of excellence in academics, athletics, professional career accomplishments, and service), 2000

University of Louisville Alumni Scholar for Research Award, 1998-2000

University of Louisville Presidential Young Investigator Award, 1994

Named Lutz Microfabrication Cleanroom Director, 1994

University of Cincinnati Graduate Research Scholarship, 1987-1992

University of Cincinnati URC Summer Research Fellowship, 1988

Who's Who Among College Students, 1979

NCAA Post Graduate Scholarship, 1979-1980

Speed Scientific School Alumni Award, 1977

Samuel T. Fife Award, 1976

Ed Kallay Award, 1978

SCIENTIFIC AND HONORARY SOCIETIES

Institute of Electrical and Electronic Engineers (IEEE), American Society for Engineering Education (ASEE), Instrument Society of America (ISA), Sigma Xi Scientific Research Society, Eta Kappa Nu Honorary Society, Tau Beta Pi Honorary Society

OTHER RELEVANT INFORMATION

Equipment Donations of over \$2,000,000 since 1992

Reviewer for *Analytica Chimica Acta*, 2002

Reviewer, Proposal for The Petroleum Research Fund, *American Chemical Society*, 2002

Reviewer for the *North Carolina Biotechnology Center, Science and Technology Program*, 2001

Reviewer Fundamentals of Microelectronic Circuit Design and Analysis by Gerold Neudeck, 2001

Reviewer for *2000 ASME Conf. BioMEMS Session*, 2000

Reviewer for *Engineering Design and Automation Journal*, 1997

Reviewer for *The Journal of Microelectromechanical Systems*, 1997-1998

Reviewer for *NSF Chemical Reaction Processes Program*, 1996

FPGA VLSI Program, Boston University, 1994

Microsensors and Microactuators Program, MIT, 1988

RECENT COLABORATIONS

R. Keynton (Louisville), W. Hnat (Louisville), H. Kaplan (Louisville), J. Rizzo (Harvard), D. Shire (Cornell), R. Baldwin (Louisville), R. Cohn (Louisville), John Naber (Louisville), M. Sunkara (Louisville), L. Hassebrook (Kentucky)

DOCTORAL THESIS ADVISOR

Thurman T. Henderson, University of Cincinnati, ECECS Dept.

DOCTORAL THESIS TITLE

"Development of a Fully Integrated Micromachined Piezoresistive Accelerometer/Vibration Sensor with Integral Air Damping for Condition Monitoring"

CHAKRAM S. JAYANTHI

Department of Physics, University of Louisville, Louisville, KY 40292
Email: csjaya01@gwise.louisville.edu, Telephone: (502) 852-3335

EDUCATION

University of Delhi (India)	Physics	B.Sc. (Hons) 1973
University of Delhi (India)	Physics	M.Sc (1975)
I.I.T., Delhi (India)	Physics	Ph.D. (1981)

PROFESSIONAL PREPARATION

I.C.T.P and SISSA, Trieste (Italy)	Surface Physics	Post-Doc (1981-1984)
Centre Étude Nucléaires Saclay (France)	Surface Physics	Post-Doc (1984-1985)
Max-Planck Institut, Stuttgart (Germany)	Surface Physics	Post-Doc (1985-1987)

APPOINTMENTS

Professor, Department of Physics, University of Louisville (1998-Present)
Associate Professor, University of Louisville, (1994-1998)
Assistant Professor, University of Louisville, (1989-1994)
Visiting Assistant Professor, Pennsylvania State University, (1988-1989)
Visiting Assistant Professor, Clemson University, (1987-1988)

HONORS AND AWARDS

University Scholar, University of Louisville (2000-2008)
President's Young Investigator Award, University of Louisville (1992)
National Science Talent Fellow, NCERT, India (1970-1979)

MAJOR RESEARCH INTERESTS

Theoretical studies of low-dimensional systems such as nanoclusters, nanowires/nanotubes and surfaces. Nanostructures studied include silicon clusters, carbon nanotubes, silicon nanowires, carbon nanotube-based tori, etc. Properties studied include electrical transport and electro-mechanical effects in carbon nanotubes, magnetic properties of carbon nanotube-based tori, energy gaps and optical properties of silicon clusters and Si/Ge clusters. Other research interests include the studies pertaining to surface phenomena (surface melting, surface pre-roughening, surface reconstruction, surface growth, etc.).

PUBLICATION RECORD: Author of approximately 45 refereed articles, including four review articles.

PUBLICATIONS RELEVANT TO THE PROPOSED RESEARCH

1. C.S. Jayanthi, S.Y. Wu, J. Cocks, N.S. Luo, Z.L. Xie, M. Menon and G. Yang, 'Order-N method for a Non-orthogonal Tight-Binding Hamiltonian', *Phys. Rev. B* **57**, 3799 (1998).
2. D. R. Alfonso, S.Y. Wu, C.S. Jayanthi, and E. Kaxiras, 'Linking Chemical Reactivity, Magic Numbers, and Local Electronic Properties of Clusters', *Phys. Rev. B* **59**, 7745 (1999).
3. T.W. Tombler, C. Zhou, L. Alexseyev, J. Kong, H. Dai, L. Liu, C.S. Jayanthi, M. Tang, and S.Y. Wu, 'Reversible Electromechanical Characteristics of Carbon Nanotubes under Local-Probe Manipulation', *Nature*, **405**, 769 (2000).
4. L. Liu, C.S. Jayanthi, S.Y. Wu, T.W. Tombler, C. Zhou, L. Alexseyev, J. Kong, and H. Dai, 'Controllable Reversibility of an sp^2 to sp^3 Transition of a Single-wall Nanotube under the Manipulation of an AFM tip: A Nanoscale Electromechanical Switch?' *Phys. Rev. Lett.* **84**, 4950 (2000).
5. S. Liu, C.S. Jayanthi, S.Y. Wu, X. Qin, Z. Zhang, and M.G. Lagally, 'Formation of Chain and V-Shaped Structures in the Initial Stage growth of Si/Si(100)', *Phys. Rev. B* **61**, 4421 (2000).
6. L. Liu, C.S. Jayanthi, and S.Y. Wu, 'Structural and Electronic Properties of a Carbon Nanotorus: Effects of de-localized and localized Deformation', *Phys. Rev. B* **64**, 033412-1 (2001).
8. L. Liu, C.S. Jayanthi, H. Guo, and S.Y. Wu, 'Broken Symmetry, Boundary Conditions, and Band-gap Oscillations in finite Single-wall Carbon Nanotubes', *Phys. Rev. B* **64**, 033414-1 (2001)

9. J. Kong, E. Yenilmez, T. Tombler, W. Kim, H. Dai, R. Laughlin, L. Liu, C.S. Jayanthi, and S.Y. Wu, 'Quantum Interference and Ballistic Transmission in Nanotube Electron Waveguides', *Phys Rev Lett.* **87**, 106801 (2001).
10. L.Liu, C.S. Jayanthi, and S.Y. Wu, 'Factors Responsible for the Stability and the Existence of a Clean Energy Gap of a Silicon Nanocluster', *J. Appl. Phys.* **90**, 4143 (2001).
11. M. Yu, C.S. Jayanthi, D. Drabold, and S.Y. Wu, 'Strain Relaxation Mechanisms and Local Structural Changes in $Si_{1-x}Ge_x$ alloys', *Phys. Rev. B* **64**, 16205 (2001).
12. L. Liu, C.S. Jayanthi, and S.Y. Wu, 'Manifestation of Aromaticity and its Effects on the Electronic Structure of Finite-Single-Wall Carbon Nanotubes', *Chemical Physics Letters* **357**, 91 (2002).
13. L. Liu, G.Y. Guo, C.S. Jayanthi, and S.Y. Wu, 'Colossal Paramagnetic Moments in metallic Carbon Nanotubes', *Phys. Rev. Lett.* **217206-1** (2002).

FIVE OTHER SIGNIFICANT PUBLICATIONS

1. C.S. Jayanthi, E. Tosatti, and L. Pietronero, 'Surface Melting of Copper', *Phys. Rev.* **B31**, 3456 (1981).
2. C.S. Jayanthi, H. Bilz, W. Kress and G. Benedek, 'Nature of surface phonon anomalies in noble metals', *Physical Review Letters*, **59**, 795 (1987).
3. C.S. Jayanthi, Surface Melting in a Potts-Lattice Gas Model, *Phys. Rev. Rapid Comm.*, **B44**, 427 (1991).
4. C.S. Jayanthi, S.Y. Wu and J. Cocks, 'A Real Space Green's Function Approach to the dynamics of a Vicsek fractal', *Physical Review Letters*, **69**, 1955 (1992).
5. C.S. Jayanthi, M.Tang, S.Y. Wu, J.A. Cocks, S. Yip, 'Local Analysis of Structural Instability in Stressed Lattices: Crack Nucleation in a Covalent Solid', *Physical Review Letters*, **79**, 4601, (1997).

COLLABORATORS NOT LISTED IN PUBLICATIONS (LAST 48 MONTHS): Dr. S. Sinnott, University of Florida

GRADUATE THESIS ADVISOR Prof. K.P. Jain, Indian Institute of Technology, Delhi, India

POSTDOCTORAL ADVISORS

Prof. Erio Tosatti, International School for Advanced Studies, Trieste, Italy

Prof. G. Armand (Retired), CEN Saclay, France

Prof. H. Bilz (Deceased), Max-Planck Institut Für Festkörperforschung, Stuttgart, Germany

POSTDOCTORAL SCHOLARS SPONSORED

The names of postdoctoral research associates supervised in recent years are listed below: (1) Dr. A. Kara, (2) Dr. N. S. Luo, (3) Dr. G. Yang, (4) Dr. Z.L. Xie, (5) Dr. S. Liu, (6) Dr. L. Liu, (7) Dr. M. Yu, (8) Dr. S. Shen (9) Dr. C. Basu, and (10) Dr. G.C. John.

SYNERGISTIC ACTIVITIES

Dr. Jayanthi's research integrates electronic structure methods, molecular dynamics, and computer algorithms to study a wide variety of complex systems with reduced symmetry, namely, clusters, surfaces, disordered alloys, incommensurate systems, and fractals. The goal of her research has been to understand macroscopic manifestations of physical phenomena (such as electrical transport, magnetic phenomena and fracture in solids) in terms of local electronic and structural properties of the system. Currently, Dr. Jayanthi is actively collaborating with a number of experimental and theoretical groups: Prof. H. Dai (Chemistry, Stanford University), Prof. J. Liu (Chemistry, Duke), Dr. S. Sinnott (Materials Science and Engineering, University of Florida, Gainesville), Dr. Z. Zhang (Oak-Ridge National Laboratory), Dr. M. Tang (Lawrence Livermore National Lab), Dr. G.Y. Guo (National Taiwan University), Prof. H. Guo (McGill, Canada), Prof. Fasolino at the University of Nijmegen, The Netherlands, and Prof. B. Alphenaar at the University of Louisville.

BRUCE W. ALPHENAAR

*Associate Professor of Electrical and Computer Engineering
University of Louisville, brucea@louisville.edu*

EDUCATION

Trinity College, Hartford, CT	Physics	B.S. (with honors) 1984
Yale University	Applied Physics	M.S. 1986
Yale University	Applied Physics	Ph.D. 1991
Dissertation: <i>Measurements of Inter-Channel Scattering in High Mobility Quantum Hall Conductors</i>		

PROFESSIONAL EXPERIENCE

Associate Professor, Electrical and Computer Engineering, University of Louisville	2000-date
University Scholar in Nanotechnology, University of Louisville	2000-date
Senior Researcher, Hitachi Cambridge Laboratory	1992-2000
Ph.D. Supervisor/Examiner, Department of Physics, University of Cambridge	1992-2000
Postdoctoral Researcher, Philips Research Laboratories, Eindhoven, Netherlands	1990-1992
Teaching Assistant, Yale University, Department of Applied Physics	1987-1990

AWARDS AND DISTINCTIONS

University of Louisville Scholar (2000-date); Research Associate, Corpus Christi College, University of Cambridge (1992-2000); Hitachi Managing Directors Award (1995); NASA Graduate Student Researcher Fellowship (1988-1990); McCook Mathematics Award, Trinity College (1984); Reviewer *Physical Review Letters* and *Physical Review B*; 35 refereed journal publications; 15 invited talks; 7 patents.

RELATED PUBLICATIONS

1. 'Carbon nanotubes for nanoscale spin electronics,' B. Alphenaar and S. Chakraborty, to be published in *Electron Transport in Quantum Dots*, Kluwer Academic/Plenum Publishers, Spring/Summer 2003.
2. 'Spin transport in nanotubes,' B.W. Alphenaar, K. Tsukagoshi, and M. Wagner, *Journal of Applied Physics* **89**, 6863 (2001)
3. 'Measurements of geometric enhancement factors for silicon nanopillar cathodes using a scanning tunneling microscope,' P.A. Lewis, B.W. Alphenaar, and H. Ahmed, *Appl. Phys. Lett.* **79**, 1348 (2001).
4. 'Near-infrared to visible up-conversion in a forward-biased Schottky diode with a p-doped channel,' J.S. Sandhu, J.R.A. Cleaver, A.P. Heberle, and B.W. Alphenaar, *Applied Physics Letters* **76**, 1507-1509 (2000).
5. 'Coherent transport of electron spin in a ferromagnetically contacted carbon nanotube,' K. Tsukagoshi, B.W. Alphenaar, and H. Ago, *Nature* **401**, 572-574 (1999).
6. 'Operation of logic function in a Coulomb blockade device,' K. Tsukagoshi, B.W. Alphenaar, and K. Nakazato, *Applied Physics Letters* **73**, 2515-2517 (1998).
7. 'Detection of spin-flip relaxation using quantum point contacts,' B.W. Alphenaar, H.O. Muller, and K. Tsukagoshi, *Physical Review Letters* **81**, 5628-5631 (1998).
8. 'Evidence for supercurrent quantization in interfacial Josephson junctions,' M.J. Black, B.W. Alphenaar, and H. Ahmed, *Physical Review Letters* **80**, 596-599 (1998).

RELATED RESEARCH FUNDING

1. 'Carbon Nanotube based Spin Electronic Devices,' NSF-ONR, B. Alphenaar, C. Jayanthi, and Shi-yu Wu, 10/1/02 – 9/30/05, \$450,000.
2. 'Nanofabrication of photonic crystals, nanotube spin electronics and nano electro-mechanical structures,' NASA through Western Kentucky University; R.W. Cohn and B.W. Alphenaar; 8/1/01-7/31/04; \$510,000.
3. 'Diamond Based Electronic Devices,' (pending) DOE-EPSCoR, B.W. Alphenaar, J.A. Carlisle and J. Gerbi (Argonne National Labs), 01/01/03 – 12/31/05, \$450,497.

RICHARD P. BALDWIN

Department of Physics, University of Louisville, Louisville, KY 40292
Email: rick.baldwin@louisville.edu, Telephone: (502) 852-5892

EDUCATION

Ph.D.	Analytical Chemistry	Purdue University	1976
B.A.	Chemistry	Thomas More College	1970

EMPLOYMENT

7/76-7/82	University of Louisville	Assistant Professor, Dept of Chemistry
1/81-5/81	Purdue University	Visiting Assistant Professor
7/82-7/87	University of Louisville	Associate Professor, Dept of Chemistry
1/85-5/85	Aarhus University	Visiting Lecturer
7/87-present	University of Louisville	Professor, Dept of Chemistry
7/89-12/96	University of Louisville	Chairman, Dept of Chemistry

RESEARCH INTERESTS

Electroanalytical chemistry; applications of chemically modified electrodes; bioseparations by HPLC and capillary electrophoresis.

AWARDS AND HONORS

Editor: *Analytical Chimica Acta*, 1999-present
Editorial Board: *Electroanalysis*, 1988-95
Board of Directors: Society for Electroanalytical Chemistry, 1998-2003
Professor Honoris Causa, Faculty of Chemistry, University of Bucharest, 2000-present

RECENT RESEARCH FUNDING

1. "An Integrated Monolithic Capillary Electrophoresis System with Electrochemical Detection", with Kevin Walsh and John Naber, National Science Foundation (XYZ on a Chip), \$520,000, 9/99 – 8/02.
2. "Integrated Materials Architecture: From Nanoscale Studies to Microdevice Development", Kevin Walsh (P.I.), Robert Keynton, John Naber, C.S. Jayanthi, S. Liu, S.Y. Wu, Craig Grimes, Elizabeth Dickey, Susan Sinnott, and Andrew Mason (Co-P.I.'s), NSF/Ky EPSCoR, \$439,364 (NSF) and \$513,088 (Ky) = \$952,452 Total. Walsh is P.I. of the UofL MEMS effort, Jayanthi is P.I. of the UofL Physics/Nanoscience Effort, and Grimes is the P.I. of the UK MEMS effort.
3. "Cellular Electrophysiology on a Chip", Kevin Gillis (PI, University of Missouri-Columbia), NSF (XYZ on a Chip). \$98,331 (UofL Subcontract) 10/00-9/03.

PUBLICATIONS

1. "Electrochemical Detection of Carbohydrates" (Invited Review), *J. Pharm. Biomed. Anal.*, **19**, 69-81 (1999).
2. "Recent Advances in Electrochemical Detection in CE" (Invited Review), *Electrophoresis*, **21**, 4017-4028 (2000).
3. "Electrochemical Detection of Carbohydrates at Constant Potential After HPLC and CE Separations" (Invited Chapter), in "Carbohydrate Analysis", ed. Z. El Rassi, Elsevier, in press.
4. "Fully Integrated On-Chip Electrochemical Detection for Capillary Electrophoresis in a Microfabricated Device", with T.J. Roussel Jr., M.M. Crain, V. Bathlagunda, D.J. Jackson, J. Gullapalli, J.A. Conklin, R. Pai, J.F. Naber, K.M. Walsh and R.S. Keynton, *Anal. Chem.*, **74**, 3690-3697 (2002)
5. "Synthesis and Electrochemical Characterization of a Nanocomposite Diamond Electrode" with R.C. Mani, S. Sharma, M.K. Sunkara, J. Gullapalli, R. Rao, A.M. Rao, and J.M. Cowley, *Electrochemical and Solid State Letters*, **5**, E32 (2002)

ZHI CHEN

Department of Electrical and Computer Engineering, University of Kentucky, Lexington, KY 40506
Phone: (859)257-2300 ext.268; Fax: (859)257-3092; E-mail: zhichen@engr.uky.edu

EDUCATION

Ph.D. (EE) University of Illinois at Urbana-Champaign	1999
M.S. (EE) University of Electronic Science and Technology (China)	1987
B.S. (EE) University of Electronic Science and Technology (China)	1984

PROFESSIONAL EXPERIENCE

08/01-date	Assoc. Director of Center for Micro-Magnetic Electronic Devices
07/99-date	Asst. Professor of Electrical Engineering, University of Kentucky, Lexington, KY
05/98-08/98	Member of Technical Staff, Bell Laboratories, Lucent Technologies, Orlando, Florida
01/94-07/99	Research Assistant, University of Illinois at Urbana-Champaign
01/93-12/93	Teaching and Research Assistant, Southern Illinois University at Carbondale
05/87-11/92	Assistant Professor, University of Electronic Science and Technology (China)

RESEARCH INTERESTS

Micro/nano fabrication, nano-scale devices and materials including carbon nanotube-based electronic devices, CMOS transistor reliability and deuterium processing, and integrated microsensors and microcircuits.

HONORS AND AWARDS

- NSF CAREER Award, 2001
- National Award for Invention, Ministry of Science and Technology, P. R. China, 1995.
- The Second Prize Paper Award, Industrial Automation and Control Committee, the 27th Annual Conference, IEEE Industry Application Society, USA, 1992. (*for development of reliable and drift-free humidity/moisture sensors*)
- Who's Who in America, 56th edition, 2001.
- 1998-1999 Beckman Graduate Fellowship, University of Illinois at Urbana-Champaign.

ACHIEVEMENTS

- Developed the world's first reliable and drift-free humidity/moisture sensor for trace moisture measurement (<1 ppm).
- Fabricated metal-insulator-semiconductor (MIS) structures on p-type GaAs with interface trap density of $5 \times 10^{10} \text{ cm}^{-2} \text{ eV}^{-1}$.
- Discovered new mechanism for hot-carrier-induced degradation of CMOS transistors and contributed to application of deuterium annealing to the CMOS integrated circuit manufacturing.

PUBLICATION RECORD: 32 refereed journal articles and 18 conference papers

PUBLICATIONS RELEVANT TO THE PROPOSED RESEARCH

1. W. C. Hu, L. M. Yuan, **Z. Chen**, D. W. Gong, and K. Saito, "Fabrication and Characterization of Vertically Aligned Carbon Nanotubes on Silicon Substrates Using Porous Alumina Nanotemplates," *J. Nanosci. and Nanotechnol.*, vol. 2, 203-207 (2002).
2. W. C. Hu, D. W. Gong, **Z. Chen**, L. M. Yuan, K. Saito, P. Kichambare and C. A. Grimes, "Growth of well-aligned carbon nanotube arrays on silicon substrate using porous alumina film as nano-template," *Appl. Phys. Lett.*, vol. 79, 3083-3085(2001).
3. D. W. Gong, C. A. Grimes, R. S. Singh, O. K. Varghese, **Z. Chen**, W. C. Hu and E. C. Dickey, "Titanium Oxide Nanotube Arrays Prepared By Anodic Oxidation," *J. Mater. Res.* vol. 16, 3331-3334 (2001).
4. L. Yuan, K. Saito, W. Hu and **Z. Chen**, "Ethylene flame Synthesis of well-aligned multi-walled carbon nanotubes," *Chem. Phys. Lett.* Vol. 346, 23-28 (2001).
5. **Z. Chen** and D. Gong, "Physical and electrical properties of $\text{Si}_3\text{N}_4/\text{Si}/\text{GaAs}$ metal-insulator-semiconductor structure," *J. Appl. Phys.*, vol. 90, 4205-4210 (2001).

BRUCE J. HINDS

Department of Chemical and Materials Engineering, University of Kentucky, Lexington, KY 40506-40506
E-mail: bjhinds@engr.uky.edu www.engr.uky.edu/~bjhinds, Telephone 859-2574-5507

EDUCATION:

Ph.D. Inorganic Chemistry; Northwestern University, June 1996.
M.S. Chemistry; Northwestern University, December 1992
B.S. Chemistry; Harvey Mudd College, May 1991

EXPERIENCE:

Assistant Professor: "Nanoscale Fabrication for Molecular Electronics and Chemical Separations"
Primary appointment in Materials Engineering Program with a joint appointment in the Department of Chemistry, University of Kentucky, 2001-Present
Post-Doctoral Fellowship Research: "Charge Storage Mechanism in Nano-Crystalline Si Based Single-Electron Memories" JSPS/NSF Research Fellowship, Tokyo Institute of Technology, 1998-2001. Host Professor: Shunri Oda.
Post-Doctoral Research: "Si/SiO₂ Interface Stability and Optimization." Department of Physics, North Carolina State University, 1996-1998. Host Professor: Gerald Lucovsky.
Graduate Research Thesis: "Ti-Ba-Ca-Cu-O Thin Films for Superconducting Electronics: Precursor Performance, Deposition Mechanism, Phase Formation, and Trilayer Structures by Metal-Organic Chemical Vapor Deposition." Northwestern University, 1991-1996. Ph.D. Advisor: Tobin Marks.
Undergraduate Research Thesis Project: "Kinetic Studies of Ester Hydrolysis at Transition Metal Centers within Perfluorosulfonate Films." Harvey Mudd College, 1990-1991. Advisor: Hal VanRyswyk.

AWARDS AND DISTINCTIONS:

Marubun Research Promotion Foundation Individual Research Grant, 2000
Japanese Soc. for the Promotion of Science (JSPS)/NSF Short Term Post-Doctoral Fellowship, 2000
Japanese Soc. for the Promotion of Science (JSPS)/NSF Individual Post-Doctoral Fellowship, 1998

RELATED PUBLICATIONS: (5 of 35)

1. "Control of Multiwalled Carbon Nanotube Diameter by Selective Growth on the Exposed Edge of a Thin Film Multilayer Structure" Chopra, N. Kichambare, P.D. Andrews, R. and Hinds, B.J. *Nanoletters* **2002** in press (Available as Web release, Aug. 30, <http://pubs.acs.org/journals/nalefd/index.html>)
2. "Emission Lifetime of Polarizable Charge Stored in Nano-Crystalline Si Based Single-Electron Memory" Hinds, B.J. Yamanaka, T. and Oda, S. *J. Appl. Phys.* **2001** 90(12) 6402-08.
3. "Two-Gate Transistor for the Study of Si/SiO₂ Interface in SOI Nano-Channel and Nanocrystalline Si Memory Device" Hinds, B.J.; Nishiguchi, K.; Dutta, A.; Yamanaka, T.; Hatanani, S.; Oda, S.; *Jap. J. Appl. Phys.* **2000**, 39(7B), 4637-4641.
4. "Investigation of Postoxidation Thermal Treatments of Si/SiO₂ in Relationship to the Kinetics of Amorphous Si Suboxide Decomposition" Hinds, B.J.; Wang, F.; Wolfe, D.M.; Hinkle, C.L.; Lucovsky G.; *J. Vac. Sci. Technol. B* **1998**, 16(4), 2171.
5. "Thin Films for Superconducting Electronics. Precursor Performance Issues, Deposition Mechanisms, and Superconducting Phase Formation-Processing Strategies in the Growth of Tl₂Ba₂Ca₁Cu₂O₈ Films by Metal Organic Chemical Vapor Deposition" Hinds, B. J.; McNealy, R.J.; Studebaker, D.B.; Marks, T.J.; Hogan T.P.; Schindler, J.L.; Kannewurf, C.R.; Zhang, X.F.; Miller, D.J. *J. Mater. Res.* **1997**, 12(5), 1214.

FUNDED RESEARCH ACTIVITY:

1. "Controlled Growth of Single-Walled Carbon Nanotubes for a Scalable Sub-Nanometer Lithography Process with Applications Towards Molecular Quantum Cryptology" May 2002-2005, 304k DoD EPSCOR and AFOSR
2. "Synthetic Route for Carbon Nanotube Based Permeable Membrane" April 2002-Dec. 2002 15k, Kentucky Science and Technology Corporation.

ROBERT S. KEYNTON

Associate Professor, Department of Mechanical Engineering

EDUCATION

Virginia Polytechnic Institute & State University,	Engineering Science and Mechanics, B.S., 1987
The University of Akron,	Biomedical Engineering, M.S., 1990
The University of Akron,	Biomedical Engineering, Ph.D., 1995

APPOINTMENTS

<i>Associate Professor, Mechanical Engineering, University of Louisville,</i>	7/02 to present
<i>Acting Director, Bioengineering Program, University of Louisville,</i>	8/01 to 7/02
<i>Assistant Professor, Mechanical Engineering, University of Louisville,</i>	1/99 to 6/02
<i>Assistant Professor, Biomedical Engineering, Louisiana Tech University,</i>	8/95 to 12/98
<i>Faculty Research Associate, Inst. for Micromanufacturing, Louisiana Tech University,</i>	10/95 to 12/98
<i>Adjunct Faculty, Dept. of Phys. & Biophysics, LSU Medical Ctr., Shreveport, LA</i>	9/95 to 12/98
<i>Development Engr., Design and Res. Lab, Swagelok Quick-Connect Co., Hudson, OH</i>	Summer 1988
<i>Product Development Intern, Saran and Converted Prod., Dow Chemical, Midland, MI</i>	Summer 1986
<i>Chemical Engineering Co-op, R&D, Virginia Chemicals, Inc. Portsmouth, VA</i>	1983-1985

SIGNIFICANT PUBLICATIONS

1. Baldwin, R., Roussel, T.J., Crain, M.M., Bathlagunda, V., Jackson, D.J., Gullapalli, J., Conklin, J.A., Pai, R., Naber, J.F., Walsh, K.M., and Keynton, R.S., "Fully-Integrated On-Chip Electrochemical Detection for Capillary Electrophoresis in a Microfabricated Device," *Analytical Chemistry*, 74:15:3690-3697, 2002.
2. Li, J., Friedrich, C.R., Keynton, R.S. "Design and Fabrication of a Miniaturized, Integrated, High Frequency Acoustical Lens-Transducer System," *J. of Micromech. & Microengr.*, 12:3:219-228, 2002 (Featured Paper).
3. Keynton, R.S., Rodway, N.V., Evancho, M.M., Sims, R.L., Gobin, A.S., and Rittgers, S.E., "Intimal Hyperplasia and Wall Shear in Arterial Bypass Graft Distal Anastomoses: An In Vivo Model Study," *J Biomech Engr.*, 123:464-473, 2001.
4. Keynton, R.S., Evancho, M.M., Sims, R.L., and Rittgers, S.E.: The Effect of Graft Caliber Upon Wall Shear within In Vivo Distal Vascular Anastomoses. *J Biomech. Engr.* 121: 79-88, 1999.
5. Friedrich, C., Keynton, R., Vasile, M., and Warrington, R.: Development of a Core Curriculum in Miniaturization Technologies. *J. Engr. Edu.*, Supplement, pp. 567-574, 1998.

CURRENT RESEARCH SUPPORT

1. PI, "Biomedical Nano- and Micro-Electro-Mechanical Systems," NSF-EPSCoR, 1/02-12/04, 20%, \$2,490,056.
2. PI, "The Effect of the Grade of Recipient Artery Stenosis upon the Distribution of Growth Factors in the Distal Anastomosis of Vascular Bypass Grafts," Whitaker Foundation Research Grant, PI, 4/99-9/02, 33%, \$210,000.
3. Co-PI, "Implantable Glaucoma Sensor," Kentucky Science and Technology Center, 10/02-9/05, PI - John Naber, 5% participation, \$225,000.
4. Co-PI, "Integrated Materials Architectures: From Nanoscale Studies to Microdevice Development," Department of Energy - EPSCoR, PI - Kevin Walsh, 9/00 - 8/03, 20% participation, \$952,452.
5. Co-PI, "Implementation of Deep Reactive Ion Etching Technology for the Advancement of Micro/Nano-technology Research at the University of Louisville," NSF-MRI, PI - Kevin Walsh, 9/00 - 9/02, 5% participation, \$333,000.
6. Co-PI, "XYZ-on-a-chip - An Integrated Monolithic Capillary Electrophoresis System with Electrochemical Detection," NSF, PI - Richard Baldwin, 10/99 - 12/02, 25% participation, \$520,000.

SYNERGISTIC ACTIVITIES

Developed new, cross-disciplinary, graduate level courses on MEMS and Micro Pressure and Flow Sensors for Biomedical Applications (part of an NSF Curriculum Development Grant at Louisiana Tech University).

LEI LIU

Department of Physics, University of Louisville, Louisville, KY40292
Tel. (502)852-7754; E-Mail: lei.liu@louisville.edu

EDUCATION

Ph.D.	Physics	Institute of Physics, Chinese Academy of Sciences, Beijing	1991
M.S.	Physics	Institute of Physics, Chinese Academy of Sciences, Beijing	1988
B.S.	Physics	University of Science and Technology, Heifei	1985

EXPERIENCE

07/2001 - Present	Research Assistant Professor, Department of Physics, University of Louisville
12/1998 - 6/2001	Postdoctoral Research Associate, Department of Physics, University of Louisville
07/1993 - 12/1998	Associate Professor, Department of Physics, Fudan University, Shanghai, China.
07/1991 - 07/1993	Post-Doctoral Fellow, Department of Physics, Fudan University, Shanghai, China
11/1995 - 12/1995	Visiting Scientist, International Center for Theoretical Physics, Trieste, Italy
01/1991 - 07/1991	Visiting Scholar, Dept. of Physics, Univ. of Pittsburgh, Pittsburgh, PA15232

RESEARCH INTERESTS

Effects of mechanical deformations and chemical modifications (including the modification introduced by different metal contacts and the gate voltage) on the electrical and the magnetic properties of carbon nanotube-based materials and devices.

RELEVANT PUBLICATIONS

1. Colossal paramagnetic moments in metallic carbon nanotori, Lei Liu, G. Y. Guo, C. S. Jayanthi, and S. Y. Wu, *Phys. Rev. Lett.* **88**, 217206 (2002).
2. Quantum Interference and Ballistic Transmission in Nanotube electron Waveguides, Jing Kong, Erhan Yenilmez, Thomas W. Tombler, Woong Kim, and Hongjie Dai, Robert B. Laughlin, Lei Liu, C. S. Jayanthi, and S.Y. Wu, *Phys. Rev. Lett.* **87**, 106801 (2001).
3. Structural and Electronic Properties of a Carbon Nanotorus: Effects of Non-Local Vs Local Deformations, Lei Liu, C. S. Jayanthi, and S. Y. Wu, , *Phys. Rev. B* **64**, 033412 (2001).
4. Reversible electromechanical characteristics of carbon nanotubes under local-probe manipulation, T. W. Tombler, C. Zhou, L. Alexseyev, J. Kong, H. Dai, Lei Liu, C. S. Jayanthi, M. Tang, and S. Y. Wu, *Nature* **405**, 769 (2000).
5. Controllable reversibility of an sp^2 to sp^3 transition of a single wall nanotube under the manipulation of an AFM tip: A nanoscale electromechanical switch?, Lei Liu, C. S. Jayanthi, M. Tang, S. Y. Wu, T. W. Tombler, C. Zhou, L. Alexseyev, J. Kong, and H. Dai, *Phys. Rev. Lett.* **84**, 4950 (2000).

AMY S. LOWEN

Director of Education, Louisville Science Center
Office: (502) 561-6100 Ext. 6572 alowen@louky.org

EDUCATION

SUNY, Binghamton, NY, B. A. degree, 1971

Case Western Reserve University, Cleveland, OH, M. A. degree, 1973

Case Western Reserve University, Cleveland, OH, A.B.D., Dissertation Topic: Functional Morphology of Fossil and Modern Ceropithecoide Monkeys

PROFESSIONAL EXPERIENCE

Louisville Science Center, Louisville, KY, 1978- Present

Director of Education, 2000 - present

- Responsible for all science, mathematics, and technology educational programs conducted inside and outside the Science Center.
- Coordinates Education Committee of the Board of Directors.

Director of Operations, 1993 – 2000

- Responsibilities include daily operations and educational programs of the 150,000 square foot complex that includes four floors of exhibits, an IMAX theatre and gift shop.

Associate Director of Education and Collections, 1991-1992

- Directed educational programs and teacher training, outreach, Camp-Ins, Kidspace.

Director of School and Visitor Services, 1987-1990

- Developed Discovery Labs, supervised STARLAB, floor demonstrations, volunteers, training, teacher-in-service.

Museum Educator, 1982-1987

- Created and coordinated "Falls of the Ohio" educational outreach program, Museum To Go Kits, Discovery Labs.

Researcher and Copy Writer, 1985-1987

- The Permanent Tooth and Mummy's Tomb exhibits

Naturalist, 1978-1982

SELECTED FUNDED PROJECTS

Principal Investigator, 2000

- National Institute of Health - Science Education Partnership Award (SEPA) \$1,576,000
- Health Education Rural Outreach Scientists. (Ky. – HEROS)

Project Director, 1997

- Howard Hughes Medical Institute - \$100,000
Inquiry/Explainer Immersion Project; 4-year project with J. Graham Brown School

Co-Principal Investigator, 1997

- National Science Foundation – Parental Involvement Planning Grant - \$50,000
Parent Child Interaction Project; seven city pilot program

Co-Principal Investigator, 1996

- National Science Foundation - \$795,688
THE WORLD WE CREATE permanent exhibit

Director, 1991,1993,1995 - 2000

- Title II/Eisenhower Math and Science Exemplary Funds – currently \$25,000
Annual Kentucky statewide Teacher Institute and Teacher Camp-In (1994)

Project Coordinator, 1990

- Greater Louisville Fund for the Arts - \$1,000
Visual Artist Award – creating mosaics of African American inventors

Principal Investigator, 1989

- National Science Foundation - \$450,000, Teacher Intern Project in Science – TIPS

Senior Personnel, 1988

- Department of Education - \$150,000, Teacher Intern Project in Science

NANCY POTOCZAK MILLER

High-School Teacher, Sacred Heart Academy; Telephone: (502) 589-7023

EDUCATION

- Bachelor of Science in Chemical Engineering, University of Louisville, 1983
- Master of Science in Physics, University of Louisville, 1987

PROFESSIONAL EXPERIENCE

SACRED HEART ACADEMY

August 2000-present

- Teacher of Physics and Chemistry

LOUISVILLE SCIENCE CENTER

August 1995-August 2000

- Co-Investigator for a NSF Grant, "The World We Create: A Traveling Exhibit Project."
- Research, prototype and supervise the publication of educational materials.
- Develop and present the Teacher Institute curriculum in physical science,
- Serving as faculty of record for Spalding University college credit.
- Created Rohm and Haas / Louisville Science Center Outreach Program.
- Developed Teleconferencing Outreach Program
- Researched, wrote and trained staff in physical science demonstrations.
- Researched and supervised writing of "The World We Create" exhibition script.
- Correlated interactive exhibits in "The World We Create" exhibition to scientific and mathematical standards.

UNIVERSITY OF LOUISVILLE

Adjunct Faculty

August 1991 – May 2000

Teach and administer College Physics classes with demonstrations and laboratories.

INDIANA UNIVERSITY SOUTHEAST

Adjunct Faculty August 1987 - January 1992

Taught and administered College and Engineering Physics classes with demonstrations and laboratories.

PRESENTATION ACADEMY

Physics Instructor

August 1985 - May 1987

PUBLICATIONS

1. SY Wu, ZL Xie, N Potoczak, "Calculation of the Layer Green's Function Using the Method of Resolvent Matrix", *Phys. Rev. B* 48, 14826 (1993).
2. N Potoczak, ZL Xie and SY Wu, "A Self-Consistent Calculation of the Electronic Structure of a One-Dimensional Interface", *Bull. Am. Phys. Soc.* 34, 509 (1989).
3. N Potoczak and SY Wu, "Study of Conformation Disorder in Polymer Chains Using the Recursion Method", *Bull. Am. Phys. Soc.* 33, 402 (1988).
4. N Potoczak and SY Wu, "Study of Dynamics of Polymers Using Recursion Method", *Bull. Am. Phys. Soc.* 32, 828 (1987).

JOHN F. NABER

Assistant Prof of ECE Dept. University of Louisville

EDUCATION

University of Louisville, Louisville, KY	BS	Electrical Engineering	1983
University of Louisville, Louisville, KY	Meng	Electrical Engineering	1985
Virginia Tech, Blacksburg, VA	PhD	Electrical Engineering	1992

PROFESSIONAL APPOINTMENTS

2001-present	Chief Technical Officer, Assenti LLC
2000-present	Assistant Professor (tenure appointment), Speed Scientific School, UofL
1997-2000	Assistant Professor (term appointment), Speed Scientific School, UofL
1995-1997	Lecturer, Speed Scientific School, UofL
1987-1995	Senior Member of the Technical Staff, ITT GaAs Technology Center
1985-1987	Design Engineer, General Electric Electronics Laboratory

BOOK CHAPTER

I.Bahl, D. Fisher, J.F.Naber, et al., "Gallium Arsenide IC Applications Handbook", Academic Press, San Diego, CA, ISBN: 0-12-257735-3, 1995.

PEER REVIEWED ARTICLES

1. **Electroplating for Three Dimensional Lab-on-a-Chip Electrodes and Microstructures**, Rekha S. Pai, Thomas J. Roussel, Jr., Mark M. Crain, Douglas J. Jackson, Richard P. Baldwin, Robert S. Keynton, **John F. Naber**, and Kevin M. Walsh, To be published in the BMES and IEEE International Conference on Engineering Medicine and Biology Conference, October 2002.
2. **Integration of "On-Chip" Electrochemical Detection in a Microfabricated Capillary Electrophoresis Device, for Three Dimensional Lab-on-a-Chip Electrodes and Microstructures**, Thomas J. Roussel, Jr., Mark M. Crain, Douglas J. Jackson, J. Conklin, R. Pai, J.Gullapalli, Richard P. Baldwin, Robert S. Keynton, **John F. Naber**, and Kevin M. Walsh, To be published in the BMES and IEEE International Conference on Engineering Medicine and Biology Conference, October 2002.
3. **Fully Integrated On-Chip Electrochemical Detection For Capillary Electrophoresis In a Microfabricated Device**, Richard P. Baldwin, Thomas J. Roussel, Jr., Mark M. Crain, Vijay Bathlagunda, Douglas J. Jackson, Jayadeep Gullapalli, John A. Conklin, Rekha Pai, **John F. Naber**, Kevin M. Walsh, and Robert S. Keynton. Accepted for publication, Journal of Analytical Chemistry, August 2002.
4. **Portable High Voltage Power Supply and Electrochemical Detection Circuits for Microchip Channel Electrophoresis**, Douglas J. Jackson, **John F. Naber**, Richard P. Baldwin, Thomas J. Roussel, Jr., Mark M. Crain, Kevin M. Walsh, and Robert S. Keynton. Submitted Journal of Analytical Chemistry, May 2002.
5. **Non-Invasive Myoelectrical Signal Differentiation and Processing**, J. McGinnis and J.F.Naber, Submitted IEEE Transactions on Biomedical Engineering, May 2002.

PATENTS

1. Douglas J. Jackson, **John F. Naber**, Richard P. Baldwin, Thomas J. Roussel, Jr., Mark M. Crain, Kevin M. Walsh, John Edelen and Robert S. Keynton. "An Interface Circuit for Capillary Electrophoresis Microchip Devices", USPTO Provisional Patent granted 2-8-02.
2. Douglas J. Jackson, **John F. Naber**, Richard P. Baldwin, Thomas J. Roussel, Jr., Mark M. Crain, Kevin M. Walsh and Robert S. Keynton. "An Improved Geometry for Capillary Electrophoresis Microchip Devices", USPTO Provisional Patent granted 2-8-02.
3. Douglas J. Jackson, **John F. Naber**, Richard P. Baldwin, Thomas J. Roussel, Jr., Mark M. Crain, Kevin M. Walsh and Robert S. Keynton. "An Amperometric Electrochemical Detection Circuit", USPTO Provisional Patent granted 2-8-02.

GAMINI UDAYA SUMANASEKERA

Department of Physics, University of Louisville, Louisville, KY 40292

Email: gusuma01@gwise.louisville.edu, Telephone: (502) 852-0919

PROFESSIONAL PREPARATION

University of Peradeniya, Sri-Lanka	Physics	B.S. (1981)
Indiana University	Physics	Ph.D. (1995)
University of Kentucky	Physics	Post doctoral Fellow (1995-1999)
Pennsylvania State University	Physics	Senior Research Associate (1999-2002)

APPOINTMENTS

Assistant Professor, University of Louisville, Kentucky (2002-Present)

MAJOR RESEARCH INTERESTS

Synthesis of nanostructures; transport (electrical and thermal), magnetic, optical, and structural properties of nanostructures of carbon and semiconductors; Optical properties of nanostructures of semiconductor oxides; Adsorption studies in porous media; Investigation of thermoelectric materials for high figure of merit (for refrigerators and power sources); Investigation of cathode and anode materials for high capacity rechargeable batteries; Study on 3-D photonic materials (metal and semiconductor filled synthetic opals etc.).

GRADUATE THESIS ADVISOR

Prof. J. P. Carini and Prof. D. V. Baxter, Indiana University, Bloomington

POSTDOCTORAL ADVISOR

Prof. P. C. Eklund, Pennsylvania State University

PUBLICATION RECORD

Author of about 30 articles in refereed -journals.

PUBLICATIONS MOST RELEVANT TO THE PROPOSED RESEARCH

1. G.U. Sumanasekera, B. K. Pradhan, H.E. Romero, C.W. Adu, P.C. Eklund, 'Giant Thermopower Effects from Molecular Physisorption on Carbon Nanotubes', *Phys. Rev. Lett.*, **89**, 166801 (2002).
2. B. K. Pradhan, G.U. Sumanasekera, K.A. Williams, C.W.Adu, H.E. Romero, P.C. Eklund, 'Experimental Probes of the molecular hydrogen-carbon nanotube interaction', *Physics B*, **323**, 115 (2002).
3. S. Bandow S, G. Chen, G.U. Sumanasekera, R. Gupta, M. Yudasaka, S. Iijima, P.C. Eklund, 'Diameter-selective resonant Raman scattering in double-wall carbon nanotubes', *Phys. Rev. B*, **66**, 075416 (2002).
4. H.E. Romero, G.U. Sumanasekera, G.D. Mahan, P.C. Eklund, 'Thermoelectric power of single-walled carbon nanotube films', *Phys. Rev. B*, **65**, 205410 (2002).
5. G.U. Sumanasekera, C.W. Adu, B.K. Pradhan, G. Chen, H.E. Romero, P.C. Eklund 'Thermoelectric study of hydrogen storage in carbon nanotubes', *Phys. Rev. B*, **65**, 035408 (2002).
6. B.L.V Prasad, H. Sato, T. Enoki, Y. Hishiyama, Y. Kaburagi, A.M. Rao, G.U. Sumanasekera, P.C. Eklund, 'Intercalated nanographite: Structure and electronic properties', *Phys. Rev. B*, **64**, 235407 (2001).
7. C.W. Adu, G.U. Sumanasekera, B.K. Pradhan, H.E. Romero, P.C. Eklund, 'Carbon nanotubes: A thermoelectric nano-nose', *Chem. Phys. Lett.*, **337**, 31 (2001)

SHI-YU WU

Department of Physics, University of Louisville, Louisville, KY 40292
Email: sywu0001@gwise.louisville.edu, Telephone: (502) 852-1134

PROFESSIONAL PREPARATION

National Taiwan University	Physics	B.S. (1958)
Cornell University	Physics	Ph.D. (1966)
Cornell University	Physics	Research Associate (1966-1967)
Case Western Reserve University	Physics	Research Associate (1967-1968)

APPOINTMENTS

Professor, University of Louisville, (1975-Present)
Associate Professor, University of Louisville (1972-1975)
Assistant Professor, University of Louisville (1969-1972)

VISITING POSITIONS

Resident Scientist, Insitute for Theoretical Physics, Santa Barbara, California (1997)
Visiting Professor, Universidad Autonoma de Madrid, Spain (1993)
Visiting Professor, National Taiwan University, (1996,1986)
Visiting Professor, National University, Canberra, Australia (1986)
Visiting Professor, University of North Carolina, Chapel Hill (1978; 1985-1986)
Visiting Professor, Virginia Polytechnic Institute (1978)

HONORS AND AWARDS

- Career Achievement Award for Outstanding Scholarship, Research, and Creative Activity, University of Louisville (1997-1998)
- Arts and Sciences Outstanding Research Award, University of Louisville (1992, 1993)

MAJOR RESEARCH INTERESTS

Developments of real-space electronic structure techniques (tight-binding as well as ab-initio methods), O(N) algorithms for large-scale molecular dynamics, and tool-kits for system property analysis that link the properties of complex systems to local electronic/vibrational properties. Applications have focused on the structural, electronic, mechanical, transport, and optical properties of carbon-based and silicon-based quasi-one-dimensional nanostructures.

PUBLICATION RECORD

Author of about 90 articles in refereed -journals, including five solicited review articles.

PUBLICATIONS MOST RELEVANT TO THE PROPOSED RESEARCH

1. S.Y. Wu and C.S. Jayanthi, 'Order-N Methodologies and their Applications', *Physics Reports* Vol 358/1, pages 1-74, (2002) -- *Invited Review Article*
2. L. Liu, G.Y. Guo, C.S. Jayanthi, and S.Y. Wu, 'Colossal Paramagnetic Moments in metallic Carbon Nanotori', *Phys. Rev. Lett.* 217206-1 (2002).
3. L. Liu, C.S. Jayanthi, H. Guo, and S.Y. Wu, 'Broken Symmetry, Boundary Conditions, and Band-gap Oscillations in finite Single-wall Carbon Nanotubes', *Phys. Rev. B* 64, 033414-1 (2001).
4. L. Liu, C.S. Jayanthi, S.Y. Wu, T.W. Tombler, C. Zhou, L. Alexseyev, J. Kong, and H. Dai, 'Controllable Reversibility of an sp^2 to sp^3 Transition of a Single-wall Nanotube under the Manipulation of an AFM tip: A Nanoscale Electromechanical Switch?', *Phys. Rev. Lett.* 84, 4950 (2000).
5. D. Alfonso, S.Y. Wu, C.S. Jayanthi, and E. Kaxiras, 'Linking Chemical Reactivity, Magic Numbers, and Local Electronic Properties of Clusters', *Phys. Rev. B* 59, 7745 (1999).

MING YU

Department of Physics, University of Louisville, Louisville, KY 40292
Tel. (502) 852-7754 (O); Email: m0yu0001@gwise.louisville.edu

EDUCATION

Ph.D.	Condensed Matter Physics	Hokkaido Institute of Technology, Japan	Mar. 1995
M.S.	Solid State Physics	Northeastern University, China	Jan. 1987
B.S.	Theoretical Physics	Liaoning University, China	Jul. 1982

Ph. D Advisor: Professor Y. Kakehashi, Hokkaido Institute of Technology, Japan
Postdoctoral Advisors: Professor P. Fulde, Max-Planck-Institute, Dresden, Germany
Dr. Sergio E. Ulloa and Dr. David A. Drabold, Ohio University

RESEARCH & TEACHING EXPERIENCE

- **Research Assistant Professor, Aug. 2001 – Present,**
Department of Physics, University of Louisville
- **Postdoctoral Research Associate, March 1999 – July 2001**
Department of Physics, University of Louisville
- **Postdoctoral Research Associate, May 1997 – Feb. 1999**
Department of Physics and Astronomy, Ohio University
- **Visiting Scientist, Apr. 1995 - Apr. 1997**
Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany
- **Lecturer, Feb. 1987 – Sep. 1991**
Department of Physics, Northeastern University, Shenyang, China

RESEARCH INTEREST

LCAO-based large-scale molecular dynamics simulations of low-dimensional silicon-based systems such as Si nanoclusters, Si nanowires, Si (111)-7x7, and Si (100)-C4x2 and their structural, electronic, and optical properties. The LCAO-based large-scale molecular dynamics incorporates the self-consistency in the charge-transfer and multi-center (electron-electron and electron-ion) interactions via environment-dependent terms.

PUBLICATIONS

1. Strain Relaxation and Local Structural Changes in Si_{1-x}Gex Alloys, Ming Yu, D. A. Drabold, C. S. Jayanthi, and S.Y. Wu Phys. Rev. **B64**, 165205, (2001).
2. Local Basis Quasiparticle Calculations for the Dielectric Response Function of Si Clusters, Ming Yu, Sergio E. Ulloa, and David A. Drabold, Phys. Rev. **B61**, 2626 (2000).
3. Local basis GW calculations and the dielectric response of Si and C clusters, Ming Yu, Sergio E. Ulloa, and Sang H. Yang, Mat. Res. Soc. Symp. Proc. **579**, (2000).
4. Density Dependence of the Structural and Electronic Properties of Amorphous GaN, Ming Yu and David A. Drabold, Solid States Communication, **108**, 413 (1998)
5. Electron Correlation in First-row Homonuclear Diatomic Molecules: Charge Fluctuations and Correlation Strength in Chemical Bonds, M. Yu, M. Dolg, P. Fulde, and H. Stoll, Inter. J of Quantum. Chem. **67**, 157, (1998).

HONORS & AWARDS

- Excellent Thesis, Hokkaido Institute of Technology, Japan, 1995
- Young Physicist Fellowship, The 3rd Asia-Pacific Physics Conference, 1988
- Excellent Thesis, Liaoning University, China, 1982

2 Cluster Research Description

2.1 Overall Cluster Summary - **High Energy Theoretical Physics**

Through the activities supported by the proposed project, we hope to establish the University of Kentucky as a major center for high-energy theoretical physics research. These activities will aim to produce important and internationally recognized scientific results, attract scientists and students of the highest calibre to Kentucky, support a world-class program of lectures, seminars, and workshops, and provide educational opportunities for students from the high school through postdoctoral levels. Achieving these goals will require an acceleration of our research and educational efforts at all levels.

Three co-PIs, Profs. Alfred Shapere, Sumit Das, and Susan Gardner of the University of Kentucky, along with Prof. Sharmanthie Fernando of Northern Kentucky University, will conduct and supervise an extensive program of research in string theory, gauge theories, astrophysics, and Standard Model phenomenology. Specific research areas will include studies of the theory and phenomenology of black hole production and decay; explorations of the connections between strings, quantum gravity, and gauge theories; development of phenomenological tests of discrete symmetries and probes of new physics beyond the Standard Model; and theoretical investigations of gauge theories and supersymmetry.

It is important to emphasize the unique nature of successful research efforts in our field: much progress is made interactively and collaboratively, and new results must be rapidly disseminated in an increasingly competitive and fast-moving environment. These factors give groups with several postdocs and students a significant advantage. The bulk of our funding request is therefore for personnel, at the undergraduate through senior levels.

Each of the three Investigators will supervise one postdoctoral associate. Experienced postdoctoral researchers trained at the world's top graduate programs will be crucial in carrying out the investigations full-time, and will help to train the research group in the most up-to-date analytical techniques. Four graduate students, two each to be supervised by Das and Shapere, will work closely with faculty and postdocs and play an integral role in the research effort. Undergraduates will also contribute to the research effort in summer months. Postdocs will assist in training these students, as part of the educational mission of the project.

An active visitors' program will bring in a steady stream of top physicists per year from national labs and centers as well as international institutions. Their visits will give us access to the latest techniques and results in our rapidly-developing research areas, enable collaborations with top scientists from leading institutions, and give these scientists opportunities to observe the high quality of our research program first-hand. Short-term visitors will give seminars and interact intensively with the research group. A series of high-profile longer-term visits will greatly increase the visibility of our program and establish collaborative and cooperative ties with these scientists and their top institutions. Longer-term visitors will collaborate with the co-PIs and postdocs, and will be encouraged to give a series of lectures.

Extensive travel to conferences, workshops, national labs, and institutions will also keep

us abreast of the latest research, raise our visibility, and support the development of collaborations with other research groups around the world.

The grant will also support the research of Prof. Sharmanthie Fernando, an Assistant Professor at Northern Kentucky University (NKU) who is an active researcher in our field. By supporting Prof. Fernando as an active participant in the proposed effort, we will establish strong new ties between our respective institutions and lay the groundwork for a continuing collaborative relationship with Prof. Fernando and her associates at NKU.

Educational and outreach activities will include regular presentations of frontier research in high-energy physics to students at Kentucky high schools and 4-year colleges, a series of public lectures by distinguished physicists, and a black hole course aimed at beginning undergraduates and community members. Training of graduate students and postdocs, and research projects for two undergraduates per year, will serve both educational and scientific functions.

2.2 Goals

The overarching scientific goal of the proposed project is to explore and elucidate theoretical and phenomenological aspects of theories of elementary particles, quantum gravity, and string theory. Some of the specific aims of the research component of the project are

- to improve our understanding of the formation, structure, and decay of black holes.
- to study Hawking evaporation and related properties of quantum gravity in the context of string theory.
- to explore holographic relationships between quantum field theories, quantum gravity, and string theory.
- to propose new phenomenological tests of low-scale gravity.
- to improve existing limits on the fundamental scale of quantum gravity.
- to propose and analyze tests of discrete symmetry violation and new physics in heavy meson systems.

The educational goals of the proposed project are

- to create diverse educational opportunities for students, teachers, and the general public to learn about high-energy physics directly from its practitioners;
- to enhance the quality of undergraduate and graduate physics education in Kentucky, by providing students with exciting and meaningful research experiences;
- to encourage and inspire high school students and beginning college students to consider making a career in science;

- to expose students, teachers, and the general public to the frontiers of physics, by giving lectures and conducting discussions on topics related to the proposed research at local high schools and small colleges;
- to provide beginning undergraduates and community members with in-depth opportunities for learning about current research topics, by designing and offering a nontechnical introductory night course on the physics of black holes and by organizing a series of public lectures by some of the world's most distinguished physicists;
- to promote greater public understanding of physics and the scientific process in an area with one of the lowest scientific literacy rates in the U.S.

The overall goal of the project is to raise the profile and productivity of our research and educational program to a level of international prominence and competitiveness. In pursuit of this goal, in addition to the activities described above, we aim

- to establish strong cooperative and collaborative ties with the world's leading laboratories and centers for high-energy physics research, through supported travel to these sites and an active program to bring top scientists from these centers to Kentucky.
- to establish the suitability of the University of Kentucky as a site for a planned Center for High Energy Theoretical Physics.

2.3 Introduction

High energy theoretical physics has been one of the most active frontiers of research in all of science since the 70s, yet it is a relatively new endeavor in the state of Kentucky. Since 1994, the Department of Physics at the University of Kentucky (UK) has added five new faculty members in this field. Three of these faculty members, Sumit Das, Susan Gardner, and Alfred Shapere, are engaged in research at the highest experimentally accessible energies and beyond, aiming through analytic techniques to uncover the fundamental structure of matter and energy. Their research programs are a major new thrust for the Department, where work in high-energy physics was previously confined to lower energy scales and oriented towards computational approaches.

Because of the newness of this research program, the investigators have yet to obtain traditional funding beyond a subsistence level. In order to attract a level of long-term funding sufficient to carry out research in this highly competitive and rapidly developing field, it will first be necessary to establish the viability of Kentucky as a major center for high-energy physics research, increase the collaborative and cooperative ties of this research group to other groups around the world, and enhance the international reputation of the program.

These are the goals for the EPSCoR project initiated in 2000, for which the present proposal is a renewal request. Thanks to the EPSCoR program, we have already made substantial progress towards achieving these goals, that we could not have made in any

other way. We have hired a well-known faculty member and an excellent group of postdocs, and research activity for the group is at an all-time high. In the Progress Report section below, we discuss in detail our achievements under the EPSCoR grant so far.

Our achievements over the past three years have brought unprecedented recognition to Kentucky's new efforts in high-energy theoretical physics. However, the time has come to take our program to the next level. With additional support over the next three years, we believe that we can become a truly important center for high-energy physics, that will be capable of sustaining the most active research and educational programs in the region. While continuing to produce important and internationally recognized scientific results, we hope to attract a steady stream of scientists of the highest calibre to Kentucky, both as short-term visitors and in longer-term capacities, as graduate students, postdocs, and senior sabbatical visitors. We also intend to support a world-class program of lectures, seminars, and workshops, and to provide extensive educational opportunities for students from the high school through postdoctoral levels.

By demonstrating the viability and success of a vigorous research effort in the above-described areas, the proposed activities will lay the groundwork for the formal establishment of a Center for High-energy Theoretical Physics at the University of Kentucky, which we aim to achieve with University and federal support by 2006. The proposed Center will support well-coordinated research efforts in various areas of high energy theory and will have a vigorous visiting program centered on extended workshops on specific topics. The Center will provide dedicated offices and discussion space for students, postdocs, and visitors. Similar, highly successful institutes at the University of California at Santa Barbara, U. Michigan, U. Minnesota, and Rutgers will serve as models for our Center, which will be the first of its kind in this part of the U.S., and will serve as a regional focus of activity for an area that includes Ohio, Indiana, Tennessee, and West Virginia.

2.3.1 Progress Report

The following is a progress report on the work performed by the co-PIs involved in the theoretical part of the project during the previous cycle of DOE-EPSCoR funding, which began July 1, 2000.

Among our achievements since 2000, perhaps the most significant was the hiring of Sumit Das, formerly of the Tata Institute of Fundamental Research in Bombay, India. Das is a leading string theorist and winner of India's most prestigious national science award, the Bhatnagar Prize. His hiring has caused a stir throughout the international string theory community, and has done more than anything else we have accomplished during the past three years to increase our visibility.

Attracting Das away from the top string theory institute in Asia was no simple matter, and EPSCoR played a key role. Thanks to EPSCoR, we were able to offer Das a substantial startup package, which included the hiring of two postdocs of his choice. Without postdocs, Das could not have maintained a research program at the level to which he was accustomed at the Tata Institute, and it is highly unlikely that he would have come. In fact, he has been

able to attract postdocs of the highest caliber, Jeremy Michelson and Partha Mukhopadhyay, who are students of two world's most well-known string theorists, Andrew Strominger and Ashoke Sen.

Das's presence has injected tremendous new energy into our research effort. His 3 papers since his arrival in January 2002 on cutting-edge topics in string theory have already received wide notice (one of them has already earned 50 citations). He has established or re-established collaborations with several top US-based string theorists since arriving, and has brought in a steady stream of well-known visitors, including Jeff Harvey, Ashoke Sen, and Leonard Susskind. His teaching is so inspiring that four out of six of the students in his quantum field theory course want to do their doctoral research with him.

Our other research achievements of the last 3 years have been discussed in detail in the Project Description. Here we enumerate some of the highlights:

- Shapere, with collaborator Jonathan Feng of UC Irvine, proposed that ultra-high-energy cosmic ray events could be used to probe the structure of possible higher dimensions. This work has received well over 50 scientific citations and has been the subject of articles in Physical Review Focus, Nature, Science News, USA Today, and other publications[6].
- With additional collaborators Luis Anchordoqui and Haim Goldberg, Shapere and Feng placed new limits on the size of the higher dimensions, on the scale of higher-dimensional gravity [9], and on the physics of high-energy neutrinos [12]. In particular, the scale of gravity in higher-dimensional theories must be higher than about 2 TeV, significantly above the previous lower limit of 1.1 TeV for 3 or more extra dimensions. Limits on high-energy neutrino cross sections and cosmic ray flux were likewise improved by an order of magnitude.
- Shapere, with graduate student Ioan Popescu, succeeded in deriving an important formula conjectured by Seiberg and Witten in 1994, including an additional term which had not been previously known. Using this formula, Shapere and Popescu obtained magnetic monopole solutions, with unique and unexpected structure[27].
- Das and collaborators S.J. Rey and C. Gomez examined the Penrose limit of $AdS_m \times S^n$ spacetimes from the point of view of symmetry breaking. For a $AdS_{d+1} \times S^{\tilde{d}+1}$ background the isometry group $SO(d, 2) \times SO(\tilde{d} + 2)$ is "broken" to $SO(d) \times SO(\tilde{d}) \times H(d) \times H(\tilde{d})$ by the Penrose limit, where $H(d)$ denotes the Heisenberg group. These isometries have a natural action on the plane transverse to the plane wave, which suggested that one may regard x^+ as a holographic direction [93]. Because of the solvability of strings in these so-called pp-wave geometries and the applicability of holographic techniques, pp-waves have been the subject of much activity since the appearance of a paper by Maldacena and collaborators in February 2002. Das, Gomez, and Rey's paper appeared the following month, and has attracted over 50 citations.

- Das and Gomez [94] examined the precise manner in which the conformal algebra contracts to products of rotation and Heisenberg algebras when acting on states with large R charge J (which is taken to be positive), large conformal weight Δ and small $\Delta - J$. Using a free field approximation we showed that this process of contraction restricts all the gauge theory fields to a few low angular momentum modes, (viz the zero mode and the first nonzero mode) and ensures that fields with negative R charge do not appear in the spectrum of operators creating supergravity states. This provides an understanding of several important aspects of the proposal of [92].
- Das made use of the proposed holographic dS/CFT correspondence to study the question of thermality in de Sitter space-time. The holograms of bulk geodesic observers in terms of one point functions of dual CFT operators. If the boundary CFT is now analytically continued to lorentzian signature, these one point functions may be made constant by a coordinate transformation which induce nontrivial Bogoliubov transformations leading to thermality [74].
- Gardner proposed new tests of vector current nonconservation and second-class currents in β -decay [114].
- Gardner proposed new sources of isospin violation in K -meson decays with U. Meissner and G. Valencia [122], and studied B -meson decays with with S. Brodsky [124, 125], U. Meissner [130], and J. Tandean [131].
- Shapere graduated two PhD students, Ioan Popescu and Adel Awad. Popescu has a postdoctoral position at the British Columbia Cancer Center, and Awad is now a postdoc at the University of Cincinnati.

2.4 Proposed Research

The three co-PIs, Profs. Alfred Shapere, Sumit Das, and Susan Gardner of the University of Kentucky, along with Prof. Sharmanthie Fernando of Northern Kentucky University, will conduct and supervise an extensive program of research in string theory, gauge theories, astrophysics, and Standard Model phenomenology. Specific research areas will include studies of the theory and phenomenology of black hole production and decay; explorations of the connections between strings, quantum gravity, and gauge theories; development of phenomenological tests of discrete symmetries and probes of new physics beyond the Standard Model; and theoretical investigations of gauge theories and supersymmetry. The various research projects are grouped below by the co-PI with which they are most closely associated. Before proceeding with a detailed description of these projects, we provide some more general information about the overall goals and structure of our proposed research and educational activities.

2.4.1 Benefits of research on high-energy theoretical physics infrastructure in Kentucky

The infrastructure built by this project will include a pool of researchers trained in the analytic techniques of high-energy physics, new collaborative ties with other research institutions, and new educational ties to high schools, colleges, and the Kentucky public.

The four faculty members will provide technical education to three postdocs, four graduate students, and six undergraduates. Shapere, Das, and Gardner will each supervise one postdoc, and Shapere and Das will jointly supervise the four graduate students and six undergraduates. The technical training received by the students and postdocs will contribute significantly to the development of high-energy theoretical physics research in Kentucky.

Extensive travel to top research institutions and numerous visits by scientists based at these institutions will strengthen our ties with these institutions and heighten our visibility.

The participation of Prof. Sharmantie Fernando will establish new cooperative and collaborative ties with the high-energy physics research program at Northern Kentucky University.

The proposed activities will also lay the groundwork for establishment of the Kentucky Center for Theoretical Physics, which with university support we hope to inaugurate by the end of the term of this grant. The proposed Center will include dedicated office space, secretarial help, computational resources, and videoconferencing facilities.

2.4.2 Estimate of unexpended funds that will remain at the end of June 2003

Of the original DOE grant of \$325,667 for the 3-year period beginning July 1, 2000, we expect \$110,000 to remain unspent by June 30, 2003. These residual funds are earmarked for salaries through August 31, 2004 of two postdocs, Jeremy Michelson and Partha Mukhopadhyay. These two positions were part of Sumit Das's hiring package. Because Das did not accept our faculty offer until late in Year 1, after the conclusion of the postdoc hiring season, these postdocs could not be hired until Year 2, to begin working in Year 3. Difficulties in obtaining a visa for one of the postdocs has further delayed spending. We plan to request a no-cost extension for these funds until August 31, 2004 in order to pay these two postdocs through the end of their two-year terms.

2.4.3 DOE National Lab affiliations and cooperative work

The Investigators plan to use some of the requested travel funds to solidify ties with research groups at the Stanford Linear Accelerator Center (SLAC) and Fermilab, and expect to collectively make at least 3 visits per year to these DOE labs. We also plan to invite a number of top researchers from these labs for visits, including Stanley Brodsky, Bogdan Dobrescu, Joanne Hewett, Shamit Kachru, Joseph Lykken, Helen Quinn, Thomas Rizzo, and Eva Silverstein. Brodsky, Kachru, and Silverstein have confirmed their willingness to visit.

2.4.4 Educational and outreach activities

A significant outreach and educational component of the project will aim to create diverse educational opportunities for students, teachers, and the general public to learn about high-energy physics directly from its practitioners. Various activities will be aimed at students from the high school through the postdoctoral levels.

Through a program of presentations at area colleges and high schools, Kentucky students will be exposed to frontier physics research (and particularly to topics related to research supported under this grant). Two public lectures per year will also provide students and community members with opportunities to learn about high-energy physics research, in this case from some of its most distinguished practitioners. A new night course on black holes, to be developed and first offered in Year 1, will provide an opportunity for beginning undergraduates and community members to acquire in-depth knowledge about a subject that is as fascinating to researchers as it is to many nonscientists. Research opportunities for undergraduate and graduate students will enhance the quality of undergraduate and graduate physics education in Kentucky, and provide these students with opportunities to directly experience the excitement of frontier research.

To support many of these activities, and as a further form of outreach, we plan to construct and maintain a website describing our research activities in a manner accessible to the general public and containing supporting and follow-up material for students and teachers involved in the visits to colleges and high schools.

Through these outreach activities, we hope to help science students and their teachers understand better what theoretical physicists do, to convey some of the excitement of frontier research and some appreciation of the problems waiting to be solved, to inspire talented students to consider pursuing careers in science, and to promote greater public understanding of physics and the scientific process in an area with one of the lowest scientific literacy rates in the U.S.

Traditionally underrepresented groups are well-represented by the supported personnel: among the four investigators, two are women and two are of South Asian origin; also, one graduate student is of Hispanic origin.

2.4.5 Changes in Size and Scope

We summarize here the changes in senior personnel, size, and scope relative to the initial three-year phase of the grant.

Personnel changes: The faculty member listed on the original proposal as “To-Be-Named” is Sumit R. Das. He began working at UK in January 2002. Michael Crescimanno left Berea College in 2001 and moved to Youngstown State University in Ohio. Sharmanthie Fernando of Northern Kentucky University will join the effort in 2003. This proposal only covers the theoretical subcluster of the original proposal. The experimental nuclear subcluster included in the initial phase, consisting of Daniel Dale (PI), Wolfgang Korsch (co-PI), and Brian Milbrath, is not participating in this renewal proposal.

Changes in size: We are requesting funding for four graduate students over the term of the grant, in response to expanded research needs, student demand, and as part of our expanded educational effort. We are also requesting additional funds to support a significantly expanded visitors' program.

Changes in scope: We are proposing a greatly increased educational effort, that will reach high school students, teachers, and the general public.

2.4.6 Research of Alfred Shapere

Alfred Shapere will conduct and supervise research aimed at exploring the structure, theoretical predictions, and phenomenological implications of gauge theories, quantum gravity, and string theory.

Continuing work will study the possibility that black holes could be produced by neutrino cosmic rays, and the prospects for observing their effects at existing and planned facilities. Observation of an enhanced rate of deeply-penetrating cosmic ray showers, with specific characteristics and statistics, could provide the first experimental evidence for the existence of extra dimensions. Nonobservation of excess events will set new lower bounds on the scale of higher-dimensional gravity. Theoretical uncertainties in calculations of black hole production rates will be addressed within the frameworks of classical and quantum gravity, extra-dimensional scenarios, and string theory.

Research on 4D gauge theories with extended supersymmetry will continue, with particular attention to the structure of supersymmetric solitons. Also, a search will be made for non-supersymmetric solitons, predicted to exist by string theory. This work could provide a direct field-theoretic derivation of the spectrum of supersymmetric states in these theories, which thus far has only been available from string theory, and new insights into the dynamics of QCD.

In the area of string theory, a study now in progress of the Matrix theory for pp-wave backgrounds has yielded a large class of new vacuum solutions. The interpretation and significance of these solutions, including the possibility that they represent a new phase of strings, will be investigated.

Finally, the physics of nonabelian antisymmetric tensor fields will be studied, their dynamics, quantization, and possible applications to string theory and Standard Model phenomenology.

Collaborators in these various projects will include Sumit Das, Herbert Morales, and Partha Mukhopadhyay (University of Kentucky), Philip Argyres (University of Cincinnati), Jonathan Feng (UC Irvine), Luis Anchordoqui, Haim Goldberg (Northeastern Univ.), and Ioan Popescu.

Background

In phenomenological scenarios with TeV-scale gravity, it has been noted that black holes could be produced in high-energy particle collisions [1, 2, 3, 4, 5]. A paper by Shapere and

Jonathan Feng in September 2001 [6] pointed out that cosmic rays could produce black holes, since their center-of-mass energies can exceed 100 TeV, far above the threshold for black hole production in these scenarios.

Neutrino cosmic rays in particular could produce black holes at significant rates, which would decay almost instantly into spectacular hadron-like showers. Because of the short mean free path of hadrons through the atmosphere, hadronic cosmic rays typically initiate showers at the very top of the atmosphere. Background from hadronic showers can be almost completely eliminated by searching for low-altitude quasi-horizontal showers, in which the cosmic ray primary must penetrate several atmospheric depths. In fact, the only conventional candidates able to produce such showers are ultra-high-energy neutrinos, which have such small cross-sections that they are expected to initiate showers at equal rates for all atmospheric depths. Searches for such showers have been underway for several years, and no events above background have yet been detected.

Feng and Shapere studied the prospects for observing black holes produced by neutrino cosmic rays at the Pierre Auger Observatory, which when fully operation in 2003 will cover 3000 km² and have 30 times the aperture of the Akeno Giant Air Shower Array (AGASA), the largest currently operating ground-based cosmic ray detector. They showed that, based on conservative estimates of neutrino flux, the rate for black hole production by ultra-high-energy neutrinos (10⁶ GeV and above) could be on the order of 100 times the Standard Model rate, and leading to up to 100 black hole events over 5 years' running time at Auger. On the other hand, if no events are observed in in this time period, Shapere and Feng showed that the lower limit for the scale of D -dimensional gravity M in the ADD scenario [7] will be raised above 2 TeV.

If enough candidate events are seen, it should be possible to distinguish black hole mediated events from other possible sources of enhanced event rates for deeply penetrating showers. Earth-skimming neutrinos can be used to determine whether higher event rates are due to an increased neutrino-nucleon cross section at ultra-high energies, or simply due to an unexpected rise in the neutrino flux: a higher flux will lead to a higher rate for earth-skimming neutrinos, whereas a larger cross section would decrease the earth-skimming rates by depletion. They also discussed characteristic signatures of black hole events, such as the leptonic and electromagnetic [8] components of black hole mediated showers and the expected relation between black hole mass (total shower energy) and the energies of the primary decay products.

Subsequently [9], with Luis Anchordoqui and Haim Goldberg of Northeastern, Feng and Shapere performed an analysis of existing AGASA data and showed that a lower limit on the scale of higher-dimensional gravity can already be set, of 1.3 to 1.8 TeV (depending on the number of extra dimensions). This is higher than the best previous limit of 0.6 to 1.1 TeV (depending on the dynamics of the brane model used), based on Tevatron data. A detailed analysis of the Auger detector also improved the lower limit on M_D to around 4 TeV, which will be set if no events are observed in the next five years.

Scenarios with warped extra dimensions, of the type originally proposed by Randall and Sundrum [10], were studied in [11]. Here the bounds on the scale of D -dimensional gravity

turn out not to be as stringent, although they exceed or are competitive with accelerator bounds in some parameter ranges.

A recent paper [12] combined existing Fly's Eye and AGASA data to improve by an order of magnitude the previous limits [13] on the neutrino cross section and on astrophysical neutrino fluxes at very high energies. By folding in the Fly's Eye data with our previous analyses, this paper succeeded in raising the lower bound on M_D to about 2 TeV.

These papers have been well-received by both the cosmic ray and high-energy communities, and have been well-cited by the standards of this field. The original paper by Feng and Shapere has received attention in popular and semi-technical forums, including *Physical Review Focus*, *Science News*, *Nature Science Update*, and *USA Today* [14, 15, 16, 17]. In recent months, Shapere has recently given invited seminars or colloquia at Univ. of Kentucky, U. Cincinnati, U. of Illinois Urbana, the University of Chicago, COSMO '02, Ohio State University, and the University of Florida at Gainesville. A seminar at MIT and a plenary talk at SUGRA20 in March 2003 are scheduled.

Throughout this period, Shapere has continued to study properties of $N=2$ supersymmetric gauge theories. His earlier work in this area focused on extending the work of Seiberg and Witten [18] to other gauge groups and matter multiplets [19, 20], exploring the moduli spaces of these theories and their singularities and phase boundaries [21, 22, 23, 24], and embedding these theories in string theory [26, 25].

Last year, with his graduate student Ioan Popescu, Shapere rigorously established the formula conjectured by Seiberg and Witten for the central charge in the presence of charged supersymmetric states, modulo an extra term which vanishes by inspection for specific supersymmetric solutions [27]. It is an indication of the complexity of the calculation that this result was not obtained sooner than 6 years after Seiberg and Witten's paper (not counting one previous, flawed attempt [28] and calculations in related but inequivalent contexts [29, 30]). Shapere and Popescu also derived the Bogomolnyi-Prasad-Sommerfeld (BPS) equations, for the first time directly from the superalgebra (thus ensuring supersymmetry), and found monopole and dyon solutions. The exact solvability of these theories made it possible to examine the inner structure of monopoles in unprecedented detail: their cores are hollow spherical shells of magnetic charge.

Proposed Research Neutrino Cosmic Rays and Black Holes

Over the next few years, as data arrive from Auger and other cosmic ray observatories, it will become clear whether TeV-scale gravity (at least in the ADD form) is a viable scenario. If no low-altitude, quasi-horizontal events are seen, the lower limit on the scale of gravity in these scenarios will continue to be raised farther beyond the weak scale, thus weakening their possible relevance to the hierarchy problem. On the other hand, black hole mediated neutrino cosmic ray events could provide the first evidence for the existence of extra dimensions, as well as providing an observational context for the study of microscopic black holes. If these events are observed, black holes will certainly rank among the most interesting candidates

for producing them, and it will be important to develop practical methods for distinguishing them from other possible candidates.

One approach is to study the distribution of events with respect to total energy and, by fitting it to predicted distributions, to extract from it the number of extra dimensions n and the value of M_D , as well as the minimum mass for which the Hawking picture applies accurately. With low statistics, it may be more practical to look at the characteristics of individual showers. These are expected to be similar to showers caused by large- Z nucleus primaries, though with a large electromagnetic component [8], accompanied by a few highly energetic muons. We propose to investigate in more detail both of these approaches: the statistical requirements using the energy distribution of events to determine n and M_D and the shower characteristics observable by ground-based detectors.

Dynamics of Black Hole Formation

Many of the outstanding questions and uncertainties related to black hole production are of a more theoretical nature. Still poorly understood is the process of black hole formation, although a major step forward was taken in [31], where a rigorous lower bound on the classical cross section for 4d black hole formation in 2-particle collisions was obtained. This lower bound, which is about 65% of the geometric cross section, gave strong support to the validity of our estimates. We plan to investigate the prospects for improving this lower bound in 4 dimensions and extending the calculation to higher dimensions, probably using numerical techniques. At the very least, such calculations would put our estimates of black hole production rates on much firmer ground. It is conceivable the actual cross section is considerably higher, and if a new lower bound above the geometric cross section could be established, our previous results would be correspondingly improved.

It is also essential to understand the quantum corrections to the classical picture of black hole formation and the semiclassical description of black hole evaporation, for small black holes. String theory may provide the best framework for addressing these corrections; simple scaling arguments indicate a smooth match between the string and black hole pictures [32]. In this regard, Shapere and his current graduate student Herbert Morales and have begun a project extending the work of [32]. They plan to explore in greater detail the consequences of stringy corrections to black hole production rates at energies close to the scale of higher-dimensional gravity, and to analyze their implications for the energy distribution of black hole cosmic ray events. With enough statistics to observe deviations from Hawking's semiclassical theory of black hole evaporation in the limit of small black holes, it might be possible to obtain direct observational evidence for string theory.

Potentially, strings could help us understand the physical process of black hole formation in more detail. For example, it would be useful to find a way to holographically map the process of black hole formation into a field theoretic process, possibly within the context of the AdS/CFT correspondence [39, 40]. Yet another approach could come from string field theory, where calculations of D-brane collapse could have implications for gravitational collapse. With Das and our postdoc Mukhopadhyay, we hope to explore a variety of string-based approaches to black hole formation, and to study their implications for rates of black

hole production close to the Planck scale.

Solitons of $N=2$ gauge theories

Popescu and Shapere are continuing our study of the superalgebras and solitons of $N=2$ gauge theories. We are now looking more closely at the core structure of these solutions, from the point of view of the dual effective lagrangian valid at strong gauge coupling, which is the appropriate regime close to the soliton core. This dual lagrangian can be constructed exactly (to quadratic order in derivatives), and its equations of motion appear to confirm that the simplest solutions are hollow spheres of magnetic charge localized at a characteristic radius. If this turns out to be correct, there may be direct connections to be drawn with the “empty hole” supergravity solutions of Denef [37], as well as braney structures such as enhançons. We also plan to study the interior structure of composite dyons along the lines of [38]. For example, the presence of non-normalizable singularities in some solutions could exclude them as supersymmetric states, and provide a direct field-theoretic derivation of the spectrum of such states. We also propose to look for nonsupersymmetric solutions, which have been predicted from brane solutions of Type IIB strings by Bergman [41], but which have so far not been found directly at the field theory level. Finally, we plan to extend our central charge calculation and derivation of BPS equations to include quark hypermultiplets and gauge groups beyond $SU(2)$.

Physics of Antisymmetric Tensor Fields

With Philip Argyres of Cincinnati, Das and Shapere have also begun discussing the physics of nonabelian antisymmetric tensor fields in four dimensions. The importance of understanding these fields better cannot be understated: they are expected to play a central role in little string theories [33] and in couplings of strings to stacks of NS 5-branes in IIA theory and M5-branes in M-theory. Somewhat more speculatively, but with potentially great significance, a non-abelian two-form could drive a dynamical mass-generation mechanism for vector fields, without a Higgs particle [34]. Recently [35, 36], mathematicians have proposed a way of coupling these fields to ordinary matter, defining gauge-invariant observables, and constructing dynamical lagrangians. So far, the papers on this subject which have appeared are quite mathematical, and the physical properties of two-form fields coupled in this way are far from clear. This project aims to elucidate these properties by constructing explicit lagrangians, studying their degrees of freedom in different gauge-fixing schemes, and quantizing them according to the BV procedure. Once quantized nonabelian two-form fields have been constructed explicitly, it may be possible to determine their couplings in little string theories, and to explore the possibility that these fields can provide a Higgs-free symmetry breaking mechanism.

Matrix Theory of Strings in pp-wave Geometries

Finally, a project with Das and postdoc Jeremy Michelson will explore properties of matrix models for strings in pp-wave geometries. This project is described in detail below.

2.4.7 Research of Sumit R. Das

The research described in this proposal will consist of several projects aimed at understanding space-time physics using recent insights from String Theory. The main focus is to obtain a deeper understanding of the holographic principle. One aim is to expand the detailed nature of holography in space-times other than those which are asymptotically anti de-Sitter (AdS) which include duals of noncommutative gauge theories, little string theories, plane wave backgrounds and possibly de Sitter spacetimes. In a slightly different direction, we plan to investigate solvable large- N field theories which seem to provide holographic descriptions of theories which contain gravity. An early example of this is the $c = 1$ matrix model. Recently it has been proposed that three dimensional scale invariant *vector* models are dual to theories of higher spin gauge fields in AdS_4 . We hope that the solvability of these models will provide us a better insight into holography.

Background and Past Research

The **holographic principle** [45], states that a theory of gravity in $d + 1$ dimensions is equivalent to a theory without gravity in d dimensions. This notion arose out of classic results in black hole thermodynamics. However the most concrete realization of holography were found only after the microscopic basis of Hawking radiation was understood in string theory [46, 47, 48, 49].

In a major breakthrough in 1996, Strominger and Vafa [50] found states in string theory which correspond to BPS extremal black holes with large horizons. They computed the statistical entropy of these states and found precise agreement with the semi-classical answer. Such black holes are bound states of “D-branes” [51]. The ground state of such a brane is a BPS state. The collective dynamics of a set of N parallel p -dimensional D-branes (Dp branes) is given by a theory of open strings whose end points are constrained to lie on the D-branes. At low energies this becomes a $SU(N)$ (supersymmetric) gauge theory [52]. When N is large, the system is very massive and behaves like a black brane, which becomes a black hole when the brane directions are compact. The BPS states are extremal black holes. Extremal black holes with large horizons are made out of bound states of D-branes of various kinds. The simplest example is a five dimensional generalization of the Reisner-Nordstrom black hole and was studied in [50]. The BPS nature allowed Strominger and Vafa to calculate the statistical entropy even for strong couplings where the result can be compared with semi-classical answers which are, in turn, reliable since the horizon has weak curvature. Their results were soon extended to a large class of extremal black holes.

Extremal black holes, however, have zero temperature and do not radiate. To understand the microscopic origin of Hawking radiation one needs to consider non-extremal black holes. As a first step in this direction, Samir Mathur and I investigated the low lying excitations of some number of D1 branes wrapped on a compact direction [53]. We found that these are open strings still in their lowest oscillator state (and hence reduce to massless particles) which can move along a *multiply wound* D1 brane. A BPS state has all open string moving in the

same direction, while nonextremal excitations correspond to a few of the open strings moving in the opposite direction. Such a state would decay into the extremal state by annihilation of pairs of oppositely moving open strings into a single closed string which can then escape from the brane. Since the initial state is highly degenerate, the emitted open string would appear thermal if we measure only its macroscopic properties. This would be Hawking radiation, while the inverse process would be absorption. Subsequent work of [54, 55, 56] revealed that a similar picture holds for the non-extremal excitations of the five dimensional black hole of Strominger and Vafa. Remarkably, the entropy of a slightly nonextremal system was found to be in exact agreement with the semiclassical answer, even though there is no supersymmetry which ensures that the weak coupling result can be extended to strong coupling.

Mathur and I then calculated the rate of decay of such an excited state into the ground state [58] ([54] in fact outlined such a calculation, but it was not clear how the complicated dynamics of the D-brane bound state can be tamed to perform a precise calculation). Surprisingly, this microscopic decay rate turned out to be in exact agreement with the semiclassical Hawking radiation rate. Even more remarkably, Maldacena and Strominger [59] found that the microscopic absorption rate in our work accounts for the *grey body factors* of the black hole at slightly higher energies. These results provided strong evidence in favor of a completely unitary description of black hole radiation. Klebanov [61] and Gubser, Klebanov and Tsytlin [62] found that the agreement of absorption cross-sections holds even for objects which do not have finite horizon area but are otherwise nonsingular. The simplest example is that of a set of $D3$ branes. For this system, the low energy theory is $N = 4$ supersymmetric gauge theory in $3 + 1$ dimensions. In this case the agreement is better understood in terms of known non-renormalization theorems [63].

The above developments showed that there are two rather different descriptions of absorption by a black hole. In the semiclassical description, an incoming wave falls on a black hole, part of which is scattered back and the remaining part is absorbed by the black hole. This is the standard space-time picture in general relativity. In the microscopic description one has a quantum mechanical process in which a bulk quantum is absorbed by splitting into a number of quanta of a gauge theory living on the brane worldvolume. The latter description does not involve gravity! In a major breakthrough, Maldacena used these results to make a bold conjecture [46]. He considered a low energy limit of IIB string theory in the presence of some large number (N) of $D3$ branes. The geometry near the horizon is a $AdS_5 \times S^5$ space-time with a common curvature scale $R \sim (g_s N)^{1/4} l_s$ where g_s is the string coupling and l_s is the string length. Maldacena conjectured that the low energy brane theory - which is $3 + 1$ dimensional $N = 4$ $SU(N)$ Yang Mills theory with coupling constant $g_{YM} = \sqrt{g_s}$ - is identical to Type IIB string theory in $AdS_5 \times S^5$. In the 't Hooft limit - $N \gg 1$ but $g_{YM} \ll 1$ with $g_{YM}^2 N$ finite - the string theory is classical. Furthermore, at strong coupling, $g_{YM}^2 N \gg 1$ the string theory may be truncated to supergravity.

Thus gravity in this specific background is *dual* to a gauge theory without gravity. Gubser, Klebanov and Polyakov [47] and Witten [48] found the precise connection between correlation functions of the dual descriptions and showed that the gauge theory lives on the

boundary of AdS_5 . This is therefore a concrete realization of the idea of holography. Many other examples of holography have been found and studied.

Over the past four years holography has played a crucial role in revising our notions of space and time. Processes in space-time can be viewed alternatively as processes in a gauge theory whose conceptual foundations are much better understood than gravity. At the same time holography has thrown light on strong coupling properties of gauge theories including gauge theories which are like QCD.

In fact there is a version of holography in noncritical string theory which has been known from the early 1990's. The best known example is two dimensional string theory. The corresponding holographic theory is the quantum mechanics of a $N \times N$ matrix in the double scaling limit. Here the additional dimension of the bulk theory arises out of the space of eigenvalues of the matrix. In a work with A. Jevicki [64] I showed that the density of eigenvalues is in fact the "string field", which in this case is simply a massless scalar in two dimensions. The collective field theory of this density then the full string theory. While this model is an example of holography in that an extra dimension arises from the space of matrices, it is not clear whether the matrix model is defined on some holographic screen placed in the bulk. Another version of holography is provided by the Matrix Theory formulation of M-theory [71].

Recent Research

Much of my research over the past several years has focussed on the implications of holography in various contexts. Aspects of this research which are relevant to the present project are summarized below.

Stringy exclusion principle, Giant gravitons and blown-up branes

A remarkable prediction of holography is the "stringy exclusion principle" [65] which implies that the S^n angular momenta of single particle states in a $AdS_m \times S^n$ compactification of string or M theory should be less than the quantized flux N of the n -form gauge field threading S^n . To explain this phenomenon, McGreevy, Susskind and Toumbas [66] proposed that at large angular momenta point-like supergravity modes blow up into spherical branes which are wrapped on the S^n and spinning around it. Such branes are called "giant gravitons". Since their size cannot exceed the radius of the sphere, their angular momenta also have a natural upper bound, which agrees with the predictions of the exclusion principle.

In collaboration with A. Jevicki and S.D. Mathur [67], I investigated the dynamics of giant gravitons and found the precise mechanism which leads to a gapless spectrum. We also solved the vibration spectra of these objects and found that the eigenfrequencies are *independent of the size*. The latter result gives a specific prediction for non-BPS excitations in the gauge theory at strong coupling. Such a spectrum has been recently obtained from direct open string calculation of giant gravitons in plane wave backgrounds [102].

At first sight, the delicate cancellations necessary for the giant graviton effect appear to be special to $AdS \times S$ backgrounds which also possess unbroken supersymmetries. In

a work with S. Trivedi and S. Vaidya [68], we showed that this feature is not special to such highly symmetric backgrounds. A large class of other space-times, including those which break supersymmetry, admit giant gravitons states as well. These include the near horizon geometries of extremal and near-extremal Dp branes in string theory. Furthermore, we extended the results to include giant gravitons carrying D0 brane charge.

The giant graviton effect is qualitatively similar to the dielectric effect of D0 branes placed in an external electric type (higher form) gauge field discovered by Myers [70]. However in order to have a quantitative understanding we had to (1) generalize this effect to a “magnetic moment effect”, viz. expansion of D0 branes *moving* in a magnetic type gauge field into higher dimensional branes and (2) incorporate consistently the back-reaction of the gauge field on the geometry. This was done in [68] for some interesting cases and it was found that the results from the theory of D0 branes are in agreement with those from the giant graviton picture in the relevant regime of parameters, thus providing a microscopic explanation for the giant graviton phenomenon.

Holograms of accelerated objects and cosmology on the boundary

A large body of work in holography deals with the dual description of the bulk physics as observed by an asymptotic observer. In an attempt to find the dual description of physics in other reference frames, I and A. Zelnikov [72] investigated Unruh radiation detected by accelerated observers in the bulk of AdS space. We showed that such observers correspond to *cosmological* observers in the dual boundary theory. Unruh radiation in the bulk becomes related to radiation perceived by boundary observers in the relevant boundary cosmology. Accelerated observers in AdS space-times perceive the invariant vacuum as a thermal state only when the acceleration exceeds a critical value [73]. We found the holographic explanation of this feature in terms of the nature of boundary cosmologies and observers in them for the cases of subcritical, critical and supercritical acceleration.

In a subsequent work, the above techniques were applied to *geodesic* observers in *de-Sitter* space [74]. In this case holography is rather obscure, and there are proposals [75] that the holographic theory is a *euclidean* conformal field theory living at either past or future infinity. Assuming this to be true, I calculated the holograms of bulk geodesic observers in terms of one point functions of dual CFT operators. If the boundary CFT is now analytically continued to lorentzian signature, these one point functions may be made constant by a coordinate transformation which induce nontrivial Bogoliubov transformations leading to thermality. This was interpreted as a signature of themality in the bulk. However the validity of this holographic connection is not clear at the moment (see e.g. [76]).

Noncommutative gauge theory and their gravity duals

Most examples of holography involve spacetimes which are asymptotically AdS . However there are a handful of examples where this is not the case. One such example is the near-horizon geometry of the NS 5-brane. Another example is the supergravity dual of non-commutative gauge theory. Such dual backgrounds have been proposed by Maldacena and Russo [77] and by Hashimoto and Itzhaki [78] and various aspects of this duality have been

investigated. In some situations these dual backgrounds have an *asymptotically flat* Einstein metric.

In a work with S. Kalyana Rama and S. Trivedi [79] we constructed D-instanton solutions in the bulk and provided evidence that they are dual to instantons of the noncommutative Yang-Mills theory.

One of the most important hurdles in understanding this holographic correspondence has been the fact that the gauge theory operators dual to bulk modes are not known. This is particularly confusing since the noncommutative gauge theory cannot have gauge invariant operators which are local in position space. On the other hand translation invariance requires that the states of the theory are labelled by momenta and therefore there should be gauge invariant operators with definite momentum. S.J. Rey and I [80] proposed that the relevant gauge invariant operators in noncommutative gauge theories are *open Wilson lines* constructed by Ishibashi et.al. [81]. A similar proposal was put forward by Gross, Hashimoto and Itzhaki [82] who argued that the relevant operators are *straight* Wilson lines with operators attached at one of the ends.

As a first step towards obtaining the precise form of the gauge theory operators, S. Trivedi and I [83] addressed a related question. We investigated the coupling of a *linearized* supergravity mode to a set of noncommutative branes. Using the connection of noncommutative gauge theory with matrix models we showed that the operators which couple to NS-NS supergravity modes are straight Wilson lines with operators *smeared* over it. Such operators were also obtained from loop calculations in the gauge theory by Liu [84]. Our proposal has been extended to other fields, including RR fields and was shown to be consistent with direct string theory calculations [85, 86] In a slightly different direction, supergravity couplings via open Wilson lines were used by S. Mukhi, N. Suryanarayana and I [88] to obtain an infinite subset of higher derivative stringy corrections to *ordinary* brane actions. We found perfect agreement with explicit string amplitude calculations of [89].

Strings in Plane wave backgrounds

The AdS/CFT correspondence is the best understood example of holography. However while we know a lot about the behavior of supergravity modes and their gauge theory descriptions, almost nothing is known about stringy modes. This is because it has turned out to be difficult to formulate even perturbative string theory in Ramond-Ramond backgrounds. Plane polarized waves (pp waves) provide an important exception. These are consistent backgrounds in string theory and the Green-Schwarz worldsheet action in this background becomes quadratic in light cone gauge, which makes perturbative string theory well defined [90]. Furthermore, these backgrounds may be obtained from the $AdS \times S$ backgrounds by boosting along one of the directions of the sphere and by focussing on the interior of AdS and a diameter of the S [91], an example of a Penrose limit. This latter fact has been ingeniously used by Berenstein, Maldacena and Nastase [92] to argue that the dual to string theory in the pp-wave background is simply the large R charge sector of $N = 4$ Yang-Mills theory. [92] could find operators in the Yang-Mills theory which are dual to the higher stringy modes.

In a work with C. Gomez and S.J. Rey [93] we examined the Penrose limit from the

point of view of symmetry breaking. For a $AdS_{d+1} \times S^{\bar{d}+1}$ background the isometry group $SO(d, 2) \times SO(\bar{d} + 2)$ is “broken” to $SO(d) \times SO(\bar{d}) \times H(d) \times H(\bar{d})$ by the Penrose limit, where $H(d)$ denotes the Heisenberg group. Even though the number of isometries remain the same, the generators of $H(d) \times H(\bar{d})$ do not commute with the light cone hamiltonian and are thus “broken”. There are $d + \bar{d}$ Nambu-Goldstone modes, which appear as the oscillators generating the string spectrum. These isometries have a natural action on the plane transverse to the plane wave, which suggested that one may regard x^+ as a holographic direction. In a subsequent work with C. Gomez [94], we elaborated on the symmetry breaking aspect from the point of view of the original dual gauge theory. We examined the precise manner in which the conformal algebra contracts to products of rotation and Heisenberg algebras when acting on states with large R charge J (which is taken to be positive), large conformal weight Δ and small $\Delta - J$. Using a free field approximation we showed that this process of contraction restricts all the gauge theory fields to a few low angular momentum modes, (viz the zero mode and the first nonzero mode) and ensures that fields with negative R charge do not appear in the spectrum of operators creating supergravity states. This provides an understanding of several important aspects of the proposal of [92]. The nature of holography in plane wave backgrounds, however, continues to be obscure, though there have been several suggestions [93, 95, 96, 97, 94].

Proposed Research

The proposed research project involves an in-depth investigation of crucial physical aspects of the holographic principle and related areas in String theory.

It is important to understand the nature of holography in plane wave backgrounds since this provides a concrete and controlled example of a non-AdS spacetime. The proposal of [92] is that string theory in the simplest plane wave background is *dual* to the large R sector of $N = 4$ Yang-Mills theory on $S^3 \times R$. Stated in this fashion pp-wave/CFT duality is a special case of AdS/CFT duality. In AdS/CFT duality, the gauge theory is defined on the boundary of AdS. However, in the Penrose limit one focusses on the neighborhood of a null geodesic at the *center* of AdS - the boundary is not a part of the pp-wave geometry at all. It is thus not *a priori* obvious in what sense the pp-wave/CFT duality is a holographic map. There are two aspects of this issue. The first question relates to the precise relationship of the correlation functions of large R-charge operators in “momentum” space to objects in the string theory (or for appropriate operators, supergravity) in the pp-wave background. There are proposals for such relationship for two point functions and three point functions [98]. We wish to get a better insight into holography by examining how these prescriptions follow from the standard prescriptions in the usual AdS/CFT duality. The second question relates to the issue of the dual interpretation of the RG scale parameter in the Yang-Mills theory. In the usual AdS/CFT correspondence the scale parameter is represented by the coordinate distance from the boundary in *Poincare* coordinates and a Hamilton-Jacobi form of the bulk equations of motion become the RG equations of the Yang-Mills theory. Formally one can perform a Penrose limit in Poincare coordinate system. The radial distance then becomes

a function of only the light cone time of the pp-wave. However, the null geodesic involved does not stay in the Poincare patch and the meaning of this limit is unclear. Nevertheless various authors have interpreted the light cone time as a RG scale parameter [93, 95], and Poincare limits of known RG flows seem to be consistent with this [99]. This question is not satisfactorily understood and has a bearing on the nature of holography in pp wave backgrounds. In particular, the question of duality in the Poincare patch needs to be re-examined and becomes a central issue. This has a bearing on broader questions related to extraction of physics “behind the horizon” from dual descriptions. We plan to investigate this problem by a combination of a study of correlation functions mentioned above and a better understanding of the symmetry breaking which has been studied before in [93, 94].

The second class of problems we wish to investigate involves the myers’ effect and giant gravitons. Matrix theory is well formulated in M-theory pp-wave backgrounds. Using the procedure of [100] to compactify transverse directions one may obtain a Matrix string theory which should provide a nonperturbative description of IIA strings in discrete light cone quantization. This matrix string theory has degenerate fuzzy sphere vacua which are relevant when a dimensionless combination of the RR field strength and the transverse radius becomes large. The oscillations around these would then describe a new phase of string theory. With Alfred Shapere and Jeremy Michelson we plan to investigate the physical properties of these solutions. The availability of a matrix theory formulations provides us a rare opportunity to study nontrivial vacua of string theory at the nonperturbative level.

The third direction involves dual descriptions of noncommutative string theory and little string theory [104]. Here again penrose limits of these theories may be useful [105]. In particular the problem of mode mixing which has so far prevented a good understanding of the duals of noncommutative gauge theory may be tractable in this limit. Interestingly the Penrose limit of NS five brane backgrounds lead to solvable string theories, which may shed light on other aspects of holography in such backgrounds related to boundary behavior [103]. We plan to study properties of little string theories using this fact, and hope to use recent progress in formulating theories of nonabelian two forms [106] to shed light on the structure of little string theory itself. This project will be in collaboration with Alfred Shapere and Philip Argyres.

Along a slightly different direction we wish to investigate solvable large N field theories which have dual descriptions as theories including gravity. The simplest example is the $c = 1$ matrix model mentioned above. Here the dual theory is two dimensional string theory which contains gravity, but gravity in two spacetime dimensions is not dynamical. Recently, Klebanov and Polyakov [107] have proposed that the fixed points of the three dimensional $O(N)$ vector model have dual descriptions in terms of theories of higher spin gauge fields in AdS_4 which include gravity [108]. These latter theories are *not* string theories - rather they have a single Regge trajectory. The consistency of the scheme does not require supersymmetry. However the higher spin theories are not known fully at the moment. Nevertheless the vector model is a well defined quantum field theory and may serve as a *definition* of the higher spin theory. Using techniques developed in earlier work, [109, 64] we plan to obtain the higher spin theory explicitly and study its physical properties,

e.g. thermodynamics. Our methods have the potential of determining the full action in a systematic $\frac{1}{N}$ expansion and clarify the precise nature of the holographic correspondence in this case. Antal Jevicki will be a collaborator on this project.

2.4.8 Research of Susan Gardner

My work since July, 2000 has followed different lines of inquiry; let me describe my various pursuits without regard to chronology.

Standard Model Tests in Neutron β -Decay

Searches for conserved vector current (CVC) violation and second-class currents (SCC) in nuclear β -decay experiments have spanned decades of effort. We consider a CVC test originally suggested by Gell-Mann [110]: the strength of the “weak magnetism” term of the nucleon weak current ought be given by the strength of the corresponding electromagnetic M1 transition. The SM test realized from such a comparison constrains a combination of the weak magnetism and induced tensor terms of the nucleon weak current. The induced tensor term is of odd “G-parity” — and thus is termed “second class” — and is zero in the SM [111], save for isospin-violating effects engendered by the differing mass and charge of the u and d quarks. In tests of this sort, the CVC hypothesis is tested if SCC are assumed to be zero, or, alternatively, the non-existence of SCC is tested if the CVC hypothesis is assumed to be valid.

We believe that a crisper test of the CVC hypothesis and of the non-existence of SCC can be realized via the empirical determination of the correlation coefficients of neutron β -decay; the latter are proportional to the ratio of the axial-vector to vector weak coupling constants, g_A/g_V , to leading recoil order. With the advent of the next generation of neutron-decay experiments [112, 113], the recoil-order corrections to these expressions become experimentally accessible, admitting a plurality of Standard Model (SM) tests. The measurement of both a and A , e.g., allows one to test the conserved-vector-current (CVC) hypothesis and to search for second-class currents (SCC) independently [114]. The anticipated precision of these measurements suggests that the bounds on CVC violation and SCC from studies of nuclear β -decay in the mass 12 system can be qualitatively bettered.

Isospin-Violating Effects in $K \rightarrow \pi\pi$ Decay

A detailed understanding of the rich phenomenology of $K \rightarrow \pi\pi$ decays has remained elusive despite decades of effort. Although progress has been made, the dynamical origin of the $\Delta I = 1/2$ rule, as well as the strength of CP-violating parameter $\text{Re}(\epsilon'/\epsilon)$, is not yet clear. Another, presumably related, puzzle stems from the apparent violation of Watson’s final-state theorem. Watson’s theorem emerges from unitarity and CPT-invariance, in concert with isospin symmetry, and implies that the strong phase in $K \rightarrow \pi\pi$ decay ought be given by that of $\pi\pi$ scattering. However, the S-wave $\pi\pi$ phase shift difference $\delta_0 - \delta_2$ extracted from the $K \rightarrow \pi\pi$ decay modes, using physical masses in the phase-space integrals, is about 57° [115], whereas its value from $\pi\pi$ scattering data, with the help of chiral

perturbation theory and dispersion relations, is about 45° with an uncertainty of several percent [115, 116, 117]. The assumed equality of these quantities is a consequence of isospin symmetry, so that the resolution of the discrepancy has been sought in the computation of isospin-violating effects. We show that Watson’s theorem is appropriate in $\mathcal{O}(m_d - m_u)$, so that we resolve its apparent violation through the introduction of an additional weak amplitude of $|\Delta I| = 5/2$ in character, incurred by the presence of isospin violation [118]. We find the magnitude of the $|\Delta I| = 5/2$ amplitude implied by the empirical branching ratios to be larger than expected from explicit estimates of isospin-violating strong and electromagnetic effects [119, 120]. Exploring the role of $|\Delta I| = 5/2$ transitions in the CP-violating observable ϵ'/ϵ , we determine that the presence of a $|\Delta I| = 5/2$ amplitude impacts the empirical determination of ω , the ratio of the real parts of the $|\Delta I| = 3/2$ to $|\Delta I| = 1/2$ amplitudes, and can act to decrease the SM estimate of ϵ'/ϵ , offsetting, in part, the large increase we found through the inclusion of isospin-violating effects in the matrix elements of the gluonic penguin operator [121].

The magnitude of the $|\Delta I| = 5/2$ amplitude may not be as large as our phenomenological analysis would suggest; electromagnetic effects can modify the equality between the phase shifts from $K \rightarrow \pi\pi$ decay and that of $\pi\pi$ scattering. However, including the estimated phase-shift difference from electromagnetism [119, 120] exacerbates this discrepancy. These difficulties could result from the methods used to estimate the various, unknown low-energy constants which appear. Consequently, Ulf-G. Meißner, German Valencia, and I have reconsidered Watson’s theorem in the presence of electromagnetism, in order to realize what constraints exist on the strong and electromagnetically-induced phase shifts in $K \rightarrow \pi\pi$ decay [122]. Our purpose is not a detailed numerical analysis of the various isospin-violating effects, but rather the construction of a theoretical framework which would be helpful in constraining such calculations. Nevertheless, we are able to derive consequences from the unitarity constraints which thus far have only appeared indirectly in numerical analyses [123].

Hadronic Uncertainties in B-meson decays

Another, albeit closely related, path considers the study of hadronic effects which could hamper the extraction of CKM-matrix parameters in B-meson decays. Stan Brodsky and I have shown that the presence of intrinsic charm in the hadrons’ light-cone wave functions, even at a few percent level, provides new, competitive decay mechanisms for B decays in which the tree-level contributions are Cabibbo-suppressed [124, 125]. We have shown that such contributions cannot be distinguished from “charming” penguin contributions [126, 127, 128, 129]. The intrinsic charm effect, although quantitatively elusive, is sufficiently significant, on general grounds, to impact the $B \rightarrow \pi K$ and $B \rightarrow \rho K$ branching ratios, and the associated partial rate asymmetries, in a sizeable manner, and thus the value of the CKM parameter γ extracted from a fit of the $B \rightarrow \pi K$ branching ratios.

Ulf-G. Meißner, Jusak Tandean, and I, have examined the role of $B^0(\bar{B}^0) \rightarrow \sigma\pi^0 \rightarrow \pi^+\pi^-\pi^0$ decay, as well as $B^0(\bar{B}^0) \rightarrow B^*\pi \rightarrow \pi^+\pi^-\pi^0$ decay, in the Dalitz plot analysis of $B^0(\bar{B}^0) \rightarrow \rho\pi \rightarrow \pi^+\pi^-\pi^0$ decays, employed to extract the CKM parameter α [130, 131]. The $\sigma\pi$ channel is significant because it can break the relationship between the penguin

contributions in $B \rightarrow \rho^0 \pi^0$, $B \rightarrow \rho^+ \pi^-$, and $B \rightarrow \rho^- \pi^+$ decays consequent to an assumption of isospin symmetry. Its presence thus mimics the effect of isospin violation. The σ or $f_0(400-1200)$ “meson” is a broad $I = J = 0$ enhancement driven by strong $\pi\pi$ rescattering; a suitable scalar form factor is constrained by the chiral dynamics of low-energy hadron-hadron interactions — it is rather different from the relativistic Breit-Wigner form adopted in earlier $B \rightarrow \sigma\pi$ [132] and $D \rightarrow \sigma\pi$ [133] analyses. We show that the use of this scalar form factor leads to an improved theoretical understanding of the measured ratio $\mathcal{R} \equiv \text{Br}(\bar{B}^0 \rightarrow \rho^\mp \pi^\pm) / \text{Br}(B^- \rightarrow \rho^0 \pi^-)$; fortunately, the impact on the extraction of α in $B \rightarrow \rho\pi$ appear to be small.

New Pathways to Direct CP Violation in B-meson decays

The rich resonance structure of the multiparticle ($n \geq 2$) final states accessible in heavy meson decays provides the possibility of observing direct CP violation without tagging the flavor of the decaying, neutral meson. The familiar condition for the presence of direct CP violation, $|\bar{A}_f/A_f| \neq 1$, can be met by a non-zero value of the partial rate asymmetry, so that, seemingly, one would want to distinguish empirically a decay with amplitude A_f from that of its CP-conjugate mode with amplitude \bar{A}_f . However, in neutral B , D -meson decays to self-CP-conjugate final states, direct CP violation in untagged decays may nevertheless occur. It can occur if we can separate the self-conjugate final state, via the resonances which appear, into distinct, CP-conjugate states [134]. In $B \rightarrow \pi^+ \pi^- \pi^0$ decay, e.g., the intermediate states $\rho^+ \pi^-$ and $\rho^- \pi^+$ form distinct, CP-conjugate states. As a result, the untagged decay rate contains a CP-odd amplitude combination [135]. The empirical presence of this CP-odd interference term in the untagged decay rate would be realized in the Dalitz plot as a population asymmetry, reflective of direct CP violation [134]. The conditions which permit the realization of direct CP violation in untagged modes are quite general. We need only consider self-conjugate final states whose resonances encode discrete, CP-conjugate pairs, so that we can consider not only B_d but B_s , and D decays as well. In some channels the untagged study we propose complements planned, tagged, time-dependent analyses. Nevertheless, the gain in statistical power realized in untagged versus tagged searches, i.e., roughly a factor of 2 at the B-factories and of 4 in a hadronic environment such as at CDF, argues for a more comprehensive program [136].

Proposed Research

The work we have done thus far generates continuing avenues of inquiry. We delineate two possibilities.

Hunting Direct CP Violation in Untagged B-meson Decays

Direct CP violation can exist in untagged B -meson decays to self-CP-conjugate, hadronic final states, if the resonances which appear therein form one or more pairs of distinct, CP-conjugate states. Direct CP violation in the untagged decay rate is realized as a population asymmetry across the mirror line of the Dalitz plot of the three-body decay. It is important to study the numerical size of this direct CP-violating effect, particularly in relation

to the size of the corresponding partial rate asymmetry: this is crucial to establishing the efficacy of an untagged search for direct CP violation. Jusak Tandean and I propose to do just this, in the generalized factorization approximation for the $|\Delta B| = 1$ hadronic matrix elements, for a variety of B-meson decays to three pseudoscalar mesons. Such benchmark estimates can serve various purposes. For example, the study of the population asymmetry in $B^0(\bar{B}^0) \rightarrow \rho^\pm \pi^\mp \rightarrow \pi^+ \pi^- \pi^0$ decay complements the tagged, time-dependent study of $B \rightarrow \rho \pi \rightarrow \pi^+ \pi^- \pi^0$ decay needed to determine $\sin(2\alpha)$, under an assumption of isospin symmetry [140]; if sufficiently large, it would provide an alternate pathway to the determination of the hadronic parameters which enter the isospin analysis. Moreover, the study of direct CP violation in $B^0(\bar{B}^0) \rightarrow D^{*\pm} D^\mp \rightarrow D^+ D^- \pi^0$ decay offers a direct empirical constraint on the size of penguin contributions in these decays. Once again, this is an useful complement to tagged, time-dependent analyses. Were penguins negligible, the measurement of the time-dependent asymmetry realized through the interference of $B^0 - \bar{B}^0$ mixing and direct decay determines $\sin(2\beta)$ in the SM. The equality $a_{\text{CP}}(D^* D) = a_{\text{CP}}(\psi K_s) = a_{\text{CP}}(\phi K_s) = \sin(2\beta)$ is an important prediction of the SM [141], to be confirmed or falsified through empirical study at the B-factories. Were the population asymmetry commensurate with our estimate and were $a_{\text{CP}}(D^* D)$ to deviate significantly from $a_{\text{CP}}(\psi K_s)$, we would have evidence for non-SM CP violation.

Searching for “New” Physics in $b \rightarrow ss\bar{s}$ Transitions

In the SM, $a_{\text{CP}}(\psi K_s) = a_{\text{CP}}(\phi K_s) = \sin(2\beta)$; however, current measurements show $a_{\text{CP}}(\psi K_s) - a_{\text{CP}}(\phi K_s) = \sin(2\beta)$ to differ from zero at 2.7σ [142, 143]. Various new physics models do yield a non-zero difference in a_{CP} for these modes [144]. It is worth noting that measurements of $B \rightarrow f_0(980) K_s$ decay can potentially provide more information on the $b \rightarrow ss\bar{s}$ transition. This decay, however, is theoretically less clean than $B \rightarrow \phi K_s$; in this case the contribution from the $\mathcal{O}(\lambda^2)$ suppressed $b \rightarrow su\bar{u}$ decay can be expected to make a small, rather than infinitesimal, correction. Given our knowledge of the scalar form factor, it is possible that the unwanted (small) component of the weak transition can be separated through study of $B \rightarrow f_0(980) K_s \rightarrow K^+ K^- (\pi^+ \pi^-) K_s$ decay, and it is precisely this that Ulf-G. Meißner, Jose Oller, and I plan to investigate.

2.4.9 Research of Sharmanthie Fernando

In 2+1 dimensions, supergravity theories for anti-de Sitter space can be constructed as Chern-Simons gauge theories. The AdS supergravity theories are based on AdS superalgebras. Since the AdS group in 2+1 dimensions is $\text{SO}(2,2)$ which has the factored form of $\text{SO}(2,1) \times \text{SO}(2,1)$, the super AdS group itself has the factored form $G_L \times G_R$. Supergravities based on the AdS supergroup $\text{Osp}(2,p) \times \text{Osp}(2,q)$, where p and q are integers, are referred to as $N = (p, q)$ AdS supergravities. The pure Chern-Simons supergravities were constructed by Achucarro and Townsend some time ago. In this proposal we hope to study the Chern-Simons supergravity theories along two lines as described below.

Electrically Charged Solutions in (2+1)-D anti-de Sitter Supergravities

It is interesting to try to extend pure Chern-Simons supergravity in 2+1 dimensions to include matter couplings. In the matter coupling extensions existing in the current literature, the Maxwell field is treated as a pure gauge. I plan to study models where the Maxwell field becomes dynamical. Classical solutions of such models would lead to interesting space-times including charged black holes which obey supersymmetry. Also, the boundary behavior of these models would enhance our understanding of the relation between the anti-de Sitter supergravity theory on the bulk and conformal field theory on the boundary. One of the models I plan to study is the $N = (2,0)$ charged scalar multiplet coupled to gauged $N = (2,0)$ supergravity theory. Another is the $N=2$ vector multiplet coupled to pure anti-de Sitter supergravity. In all these models I would like to study the super-conformal field theory on the boundary and the nature of the matter multiplets emerging on the boundary.

Twisted Kac-Moody Algebra and Chern-Simons Gauge Theory

Witten discovered a close connection between (2+1)-dimensional Chern-Simons theories and Wess-Zumino-Witten(WZW) models in two dimensions. Since then, many authors have studied the Chern-Simons theories, especially in connection with conformal field theories. Fernando and Mansouri studied Chern-Simons theory coupled to a source on a manifold with a boundary. The resulting boundary WZW theory leads to two copies of a "twisted" Kac-Moody algebra. The properties of this twisted Kac-Moody algebra were useful in explaining the entropy of a black hole space-time in 2+1 dimensions. It is interesting to repeat this work in the supersymmetric case. In other words, what kind of super Kac-Moody algebra arises on the boundary if a super source is coupled to the super Chern-Simons gauge theory?

2.5 Appendix: Local Collaborators

This appendix briefly describes the research of the other members of the high-energy theory group at the University of Kentucky. Its purpose is to highlight our rapidly developing program in high-energy theory, and to establish the University of Kentucky's continuing suitability as a site for the research program described in this proposal.

The theoretical high-energy physics group at the University of Kentucky consists of Sumit Das, Terrence Draper, Michael Eides, Susan Gardner, Howard Grotch, Bing-An Li, Keh-Fei Liu, and Alfred Shapere. Draper and Liu have a strong, well-funded program in lattice QCD that includes 3 postdocs, Eides and Grotch are experts in precision QED and QCD calculations, Liu and Li work on QCD and standard model phenomenology.

Our first string theory postdoc, Jeremy Michelson, formerly a postdoc at Rutgers, joined us in September. A second postdoc, Partha Mukhopadhyay, will arrive in December as soon as he completes his PhD under Ashoke Sen and obtains a US visa. These postdocs were hired under a DOE EPSCoR grant shared with Gardner and two nuclear experimentalists, which will expire in September 2003.

A graduate student, Herbert Morales, recently attended the IAS school on Prospects in Theoretical Physics (which I co-organized) and finished reading Polchinski's string theory

textbook this summer. He has recently begun doing research. Morales is Hispanic, and is currently partially supported by a one-year departmental fellowship.

Two other graduate students, Ioan Popescu and Adel Awad, completed their PhD's under Shapere's supervision in 2001. Awad, who is of north African origin, wrote his dissertation on the AdS/CFT correspondence for rotating black holes [44], and accepted a postdoctoral position with the high-energy theory group at the University of Cincinnati. Popescu chose a postdoctoral position in the medical physics group at the University of Victoria, British Columbia for family reasons, and has continued to work with me on $N=2$ supersymmetric gauge theories.

The nearest physics department to ours is located 80 miles north, at the University of Cincinnati. We have strong ties with members of this group, particularly Philip Argyres, who has been a collaborator of Shapere's for many years. Das and Shapere are currently involved in a collaboration with Argyres, as described above. Shapere has had extensive discussions over the past few months with Peter Suranyi and Rohana Wijewardhana, on the instability of black holes in Randall-Sundrum scenarios and their possible relevance to baryogenesis and early-universe cosmology.

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4 Facilities and Resources

The state-funded Center for Computational Sciences is an on-campus facility specifically for research and development, that offers faculty in the sciences at the University of Kentucky a full range of computational resources. Although the applicant may benefit from consulting services provided by the Center, the present project does not require much computational needs.

Offices for graduate students and postdoctoral associates will be provided by the Department of Physics and Astronomy

Secretarial resources and computer consultation will be provided to the applicant as needed

5 Current and Pending Support

1. Alfred D. Shapere, PI : NSF Award PHY-0071312, "Research in Quantum Field Theory and String Theory," 7/1/00 - 6/30/03, \$84,900.
2. Alfred D. Shapere (PI), Sumit R. Das, and Susan V. Gardner: "Fundamental Studies in Subatomic Physics - Theoretical," 7/1/00 - 6/30/03, \$533,470.
3. S. Gardner, PI, "Tests of Fundamental Symmetries," DOE grant #DE-FG02-96ER40989, is currently in force, at a recommended level of \$174,000, from 7/1/02 to 6/30/05.
4. Sumit R. Das, PI : NSF Proposal PHY-0244811, "Space-time properties in string theory". Total amount of request: \$393,145 for period 7/1/03 - 6/30/06 (application pending).
5. Sumit R. Das, PI : DOE Proposal to Office of Science, "Space-time properties in string theory". Total amount of request: \$393,145 for period 7/1/03 - 6/30/06 (application pending).
6. Sumit R. Das, PI and Alfred Shapere, co-PI, DOE-EPSCoR proposal under program notice 02-04, "Theoretical and Phenomenological Aspects of Black Holes and Strings". Total amount of request: \$571,417 for period 1/1/03 to 12/31/05 (application pending).
7. S. Gardner, PI, "A New Theoretical Approach to B-Meson Decays and Precision Studies of CP-Violation," pending proposal to the DOE-EPSCoR National Lab Partnership program, in conjunction with Prof. Stan Brodsky at the Stanford Linear Accelerator Center. Requested amount: \$423,358 for period 7/1/03 to 6/30/06.

6 Biographical Sketches

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- B.A. in Mathematics, Harvard University (1984)
- Ph.D. in Physics, University of California at Santa Barbara (1988)

Fellowships

- Alfred P. Sloan Fellowship, June 1995 – Dec. 1998

Employment

- Sept. 1988 – Aug. 1991: Member, Inst. for Advanced Study, Princeton, NJ.
- Sept. 1991 – Aug. 1994: Postdoctoral Associate, Cornell University.
- Aug. 1994 – Aug. 1999: Assistant Professor, University of Kentucky.
- Aug. 1999 – present: Associate Professor, University of Kentucky.

Recent Publications

1. L. A. Anchordoqui, J. L. Feng, H. Goldberg, and A. D. Shapere, "Neutrino bounds on astrophysical sources and new physics," hep-ph/0207139, to appear in Phys. Rev. D.
2. I. A. Popescu and A. D. Shapere, "Central Charge and BPS Equations of N=2 Supersymmetric Yang-Mills Theory," J. High Energy Physics 0210 (2002) 033.
3. L. A. Anchordoqui, H. Goldberg and A. D. Shapere, "Phenomenology of Randall-Sundrum black holes," arXiv:hep-ph/0204228, Phys Rev. D66 (2002) 024033, hep-ph/0204288.
4. L. A. Anchordoqui, J. L. Feng, H. Goldberg and A. D. Shapere, "Black holes from cosmic rays: Probes of extra dimensions and new limits on TeV-scale gravity," Phys.Rev. D65 (2002) 124027, hep-ph/0112247.

5. J. L. Feng and A. D. Shapere, "Black hole production by cosmic rays," Phys. Rev. Lett. 88 (2002) 021303, hep-ph/0109106.
6. A. D. Shapere and C. Vafa, "BPS structure of Argyres-Douglas superconformal theories," hep-th/9910182.

6.2 Sumit R. Das, co-PI

Sumit Ranjan Das

Professor, Department of Physics and Astronomy
University of Kentucky, Lexington, KY 40506-0055
E-mail : das@pa.uky.edu

Professional Preparation

1976 : University of Calcutta, B.Sc.(Honours) in Physics
1979 : University of Calcutta, M.Sc. in Physics
1979 - 1983 : University of Chicago, Ph.D. in Physics
1983 - 1985 : Fermilab, Post-doctoral Research Associate
1985 - 1987 : CALTECH, Post-doctoral Research Fellow

Appointments

From Jan 2002 : Professor, University of Kentucky, Lexington.
1999 - Dec 2001 : Professor, Tata Institute of Fundamental Research, Mumbai
1987-99 : Fellow, Reader and Associate Professor, Tata Institute

Awards and Honors

S.S. Bhatnagar Award, Government of India, 1998
Fellow, Indian Academy of Sciences, 1997
Valentine Telegdi Award, University of Chicago, 1980

Relevant Publications

- (1) "Realizations of Conformal and Heisenberg Algebras in the pp wave- CFT correspondence, S.R. Das and C. Gomez, *Journal of High Energy Physics* 0207 (2002) 016 [hep-th/0206062]
- (2) "Penrose limit, Spontaneous Symmetry Breaking and Holography in pp wave background" *Physical Review D* 66 (2002) 046002 [hep-th/0203164]
- (3) "Thermality in de Sitter space and holography" *Physical Review D* 66 (2002) 025018 [hep-th/0202008]
- (4) "Unruh Radiation, Holography and Boundary Cosmology", S.R. Das and A. Zelnikov, *Physical Review D* 64 (2001) 104001.
- (5) "Magnetic moments of branes and Giant Gravitons", S.R. Das, S.P. Trivedi and S. Vaidya, *Journal of High Energy Physics* 0010 (2000) 037
- (6) Open Wilson lines in Noncommutative Gauge Theory and Tomography of Holographic Dual Supergravity, S.R. Das and S.J. Rey, *Nuclear Physics B* 590 (2000) 453
- (7) Comparing decay rates for black holes and D-branes, S.R. Das and S.D. Mathur, *Nuclear Physics B* 478 (1996) 561
- (8) String Field Theory and Physical Interpretation of $d = 1$ Strings, S.R. Das and A. Jevicki, *Modern Physics Letters A* 5 (1990) 1639.

6.3 Susan V. Gardner, co-PI

Susan V. Gardner

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Home Address

3250 Pepperhill Rd.
Lexington, KY 40502
Tel: (859) 269-7997

Education

MASSACHUSETTS INSTITUTE OF TECHNOLOGY Cambridge, MA
Ph.D. degree in Theoretical Nuclear Physics, May 1988. Thesis advisor: E. J. Moniz.
CALIFORNIA INSTITUTE OF TECHNOLOGY Pasadena, CA
B.S. degree with honors in Physics and Chemistry, June, 1982.

Experience (1995 - present)

7/01-present: Associate Professor of Physics at the University of Kentucky.
[Sabbatical, Spring 2002: Theory Group, Stanford Linear Accelerator Center.]
7/95-7/01: Assistant Professor of Physics at the University of Kentucky.
8/92-7/95: Postdoctoral Fellow at the Nuclear Theory Center of Indiana University.

Recent Publications (since July, 2000).

- S. Gardner and G. Valencia, "The Impact of $|\Delta I| = 5/2$ Transitions in $K \rightarrow \pi\pi$ Decays," Phys. Rev. D **62**, 094024 (2000).
- S. Gardner and C. Zhang, "Sharpening Low-Energy, Standard-Model Tests via Correlation Coefficients in Neutron β -Decay," Phys. Rev. Lett. **86**, 5666 (2001).
- S. Gardner, Ulf-G. Meißner, and G. Valencia, "Watson's Theorem and Electromagnetism in $K \rightarrow \pi\pi$ Decay," Phys. Lett. B **508**, 44 (2001).
- S. J. Brodsky and S. Gardner, "Evading the CKM Hierarchy: Intrinsic Charm in B Decays," Phys. Rev. D **65**, 054016 (2002).
- S. Gardner and Ulf-G. Meißner, "Rescattering and Chiral Dynamics in $B \rightarrow \rho\pi$ Decay," Phys. Rev. D **65**, 094004 (2002).
- S. Gardner, "Direct CP Violation in Untagged B-Meson Decays," arXiv:hep-ph/0203152, submitted to Phys. Rev. Lett.
- Jusak Tandean and S. Gardner, "Nonresonant Contributions in $B \rightarrow \rho\pi$ Decay," Phys. Rev. D **66**, 034019 (2002).

6.4 Sharmanthie Fernando

Sharmanthie Fernando

Department of Physics and Geology

Northern Kentucky University

Highland Heights, KY 41099-1900

(859) 572-6519 [phone] fernando@nku.edu [email]

Education

- Ph.D. in Physics: 1999: University of Cincinnati, Cincinnati, Ohio, USA.
- M.Sc. in Mathematics, 1997: University of Cincinnati, Cincinnati, Ohio, USA
- M.Sc. in Physics, 1993: University of Cincinnati, Cincinnati, Ohio, USA
- B.Sc. in Mechanical Engineering, 1991: University of Moratuwa, SRI LANKA.

Employment

- Assistant Professor, Department of Physics, Northern Kentucky University, Kentucky, since 2001 August.
- Lecturer, Department of Physics, Northern Kentucky University, Kentucky, 1998-2001.: Courses taught: General Physics lecture and labs, Statics for pre engineers, Undergraduate research seminar: Total contact hours are approximately 15 hours a week.

Recent Publications

1. "Rotating Dilaton Solutions in 2+1 Dimensions". S. Fernando, NKU-00-SF1, General Relativity and Gravitation 34 (2002) 461-469.
2. "Charged Black Holes in Einstein-Born-Infeld Gravity" S. Fernando and D. Krug, to be published in General Relativity and Gravitation - Vol 35 (2003).
3. "Gravitational lensing by charged black holes", S. Fernando and Sean Roberts, NKU-01-SF1, General Relativity and Gravitation 34 (2002) 1221-1237.
4. "Twisted Kac-Moody Algebras and the Entropy of the AdS_3 Black Hole", S. Fernando and F. Mansouri, hep-th/0010153, Phys. Lett. B505 (2001), 206-214.
5. "Geodesics in Static Charged Black holes in 2+1 dimensions", Shamanthi Fernando, Don Krug and Chris Curry, preprint no. NKU-02-SF1, submitted to General Relativity and Gravitation.
6. "Mechanical Model for a Black Hole", S. Fernando, Sean Roberts and Holly Bolick, Preprint No. NKU-01-SF3.

LETTERS OF SUPPORT FOR MATERIALS RESEARCH CLUSTER

**Sandia National Laboratories**Operated for the U.S. Department of Energy by
Sandia CorporationName: Dr. Shawn Y. Lin
Title: Principal member-of-Technical-StaffP.O. Box 5800
Albuquerque, NM 87185Phone: (505) 844-8087
Fax: (505) 844-8985
Internet: slin@sandia.gov**To Whom It May Concern:**

I am writing to give my strongest and most enthusiastic support for renewing Profs. Shi-Yu Wu and C.S. Jayanthi's DOE/EPSCoR grant proposal, entitled: *"A comprehensive study of carbon-based and silicon-based quasi-one dimensional nanostructures: from the fundamental science to prototype devices"*. I am a principal member-of-technical-staff at DOE-Sandia National Laboratories and also hold Professorship at Iowa State University as well as Georgia Institute of Technology. My expertise is in the area of nano-science and nano-technology and in particular in the optical properties of *photonic band gap materials* (also known as *photonic crystals*). I currently lead Sandia's effort in developing photonic-crystal devices for optical communication and energy applications. I also head a DOE multi-laboratories initiative in Nano-Structural Photonics. I am the recipient of several awards, which include the NOVA Award from Sandia National Laboratories, the Engineer-of-the-Year award from Chinese Institute of Engineering, the Technology-of-the-Year Award from Industry Week Magazine and the R&D 100 Award, all for my contribution to photonic crystal research. I have had the opportunity to carefully evaluate Prof. Wu's proposal and also his past contributions to science and I emphatically conclude that Prof. Wu's grant proposal is truly outstanding and recommend most strongly an immediate renewal without delay.

I find the proposed research in *silicon- and carbon-based 1D nano-wires* relevant to integrated micro-systems, which are the foundation for advanced weapon systems and miniature sensing systems. The successful completion of the proposal might also lead to the direct integration of silicon microelectronics and silicon nano-photonics, an area that we are exploring for possible collaboration. The theoretical effort led by Prof. Wu is exceptionally strong, as indicated by his outstanding publications in some of the most prestigious journals such as Nature and Physical Review Letters. The experimental effort in synthesis, chemical purification, fictionalization as well as optical, electrical, and thermal characterizations are equally impressive.

Therefore, I strongly believe that the proposal is scientifically outstanding and technologically relevant to the field of nano-photonics and silicon-photonics. I recommend most strongly its renewal.

Sincerely,

Shawn Y. Lin. Nov. 07, 2002

Exceptional Service in the National Interest



Lawrence Livermore National Laboratory

Dr. Meijie Tang
P. O. Box 808, L-45
Livermore, CA 94551
Nov. 7, 2002

To DoE/EPSCoR Panelists:

This is to convey my most enthusiastic endorsement and support for the renewal of the DoE/EPSCoR proposal of Professor Jayanthi and Professor Wu entitled "A Comprehensive Study of Carbon-based and Silicon-based Quasi-One Dimensional Nanostructures: From the Fundamental Science to Prototype devices".

I am a staff scientist in the theory group of H-Division of Lawrence Livermore National Laboratory (LLNL). I have been active in the field of materials simulation and modeling for the last 10 years or so. My main focus of work is multi-scale modeling of materials properties including semiconductor, metal and nano-structured materials. In collaboration with my colleagues, we developed a new capability to study the plastic deformation in body centered cubic materials using dislocation dynamics simulations directly based on atomistic processes. This work is a key component of the Strategic Initiative project of LLNL aiming to study the mechanical properties of materials under high pressures.

I have been collaborating with the condensed matter theory group of Dr. Jayanthi and Dr. Wu at University of Louisville since 1997. We have collaborated on a wide-variety of research topics, ranging from the study of crack propagation in solids to the elucidation of the interplay between a local mechanical deformation and the transport properties of metallic single-wall carbon nanotubes. Our research collaboration has been very successful with one article published in *Nature*, two in *Physical Review Letters*, and one in a conference proceeding article.

I will be collaborating with the Louisville group on one of the projects outlined in the renewal proposal that concerns the study of the effect of local mechanical deformations on a double-wall nanotube. The purpose of this work is to investigate if the interplay between the mechanical deformation and the transport properties can enhance the electro-mechanical effect in double-walled carbon nanotubes so that nano-scale electro-mechanical switch can be realized. This indeed is a very important research in advancing the frontiers of nanotechnology. Judging from the past track record, I have every reason to believe that the projects in the renewal proposal will be just as successful as the ones in the previous grant.

In conclusion, I believe that the renewal proposal of Dr. Jayanthi and Dr. Wu deserves your most serious consideration.

Sincerely,

Meijie Tang
Staff Scientist
H-Division, Physics and Advanced Technology Directorate
Lawrence Livermore National Laboratory, Livermore, California



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November 11, 2002

To the DOE/EPSCoR Panel Members

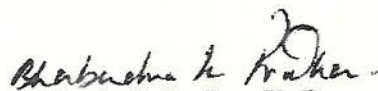
A Comprehensive Study of Carbon-Based and Silicon-Based Quasi-One-Dimensional Nanostructures: From Fundamental Properties to Prototype Devices

Dear Panelists:

I am writing this letter to endorse my support to the DOE/EPSCoR on the research proposal entitled "A Comprehensive Study of Carbon-Based and Silicon-Based Quasi-One-Dimensional Nanostructures: From Fundamental Properties to Prototype Devices". This proposal brings together a team of two theorists, an experimentalist, and an electrical engineer. Their research is important to advance the frontiers of nanotechnology as it focuses on both the fundamental understanding of different morphological forms of carbon-based and silicon-based quasi-one-dimensional nanostructures from a few nm to 50 nm and device applications (nanoscale electro-mechanical switches, nanoscale rectifiers, etc).

OUR COMPANY has a strong interest in nanoscale science and engineering and is pursuing a number of projects that focus on this area. We will be pleased to collaborate with Dr. Sumanasekera and other members of this research team. In the past, I have collaborated with Dr. Sumanasekera on several projects including "Single wall carbon nanotubes as a chemical sensor".

I wish this inter-disciplinary team every success.


Bhabendra K. Pradhan, Ph. D
Materials Scientist



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Katholieke Universiteit Nijmegen

Dr. Matesh Varma
Program Director
DoE/EPSCoR Program

Institute of
Theoretical Physics
University of Nijmegen

R e: Letter of Endorsement for Dr. Jayanthi

Dear DoE/EPSCoR Panelists

I am writing this letter to express my most enthusiastic support for the research collaboration that Dr. Jayanthi has suggested between the University of Louisville and the Institute of Theoretical Physics of the University of Nijmegen, The Netherlands.

Dr. Jayanthi and I have collaborated in the past on a few surface physics topics such as surface melting, surface phonons etc. The present collaboration aims to study the structure and formation of carbon nanorods (CNR) from a multi-wall carbon nanotube (MWCNT). In particular, we would like to understand the formation of a CNR from a MWCNT, as observed in the experiment where a CNR is irradiated with an electron beam in a high resolution scanning electron microscope. We plan to combine the complementary experiences of the Nijmegen and Louisville groups in the proposed study.

The Nijmegen group has expertise in using the grand-canonical Monte-Carlo simulations in the study of carbon-based structures based on an extension of the Brenner Potential. In particular, we have investigated the interplay between the diamond-like and graphite-like bonding in the reconstruction of (111) diamond surface.

In the present work, we plan to perform grand-canonical Monte-Carlo (GCMC) simulations to study the stability and structural properties of a CNR using the quantum-mechanical tight-binding Hamiltonian for carbon developed by the Louisville group. The GCMC technique will be ideally suited for this study as we can mimic the irradiation process by randomly removing an atom from the outer shells of a MWCNT and place it randomly in interstitial positions between shells. Various strategies for creating and removing atoms on the MWNT shells will be explored to study the formation and the stability of the carbon nanorod.

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Once the carbon nanorod structure is obtained, the nature of its inner core will be examined for the local bonding structure, local co-ordination etc so as to shed light on the results of TEM and HRTEM studies which suggest a solid amorphous core for the CNR

Dr. Jayanthi plans to visit Nijmegen for three months from June 15, 2003 to September 15, 2003. During this period, Dr Jayanthi will familiarize herself with our GCMC code and interface it to her tight-binding code. It is anticipated that we may have to meet briefly again in 2004 to wrap-up the work.

I sincerely hope that you will be able to find funds to support the research collaboration outlined in this letter.

If you need any additional clarification, please do not hesitate to contact me.

Sincerely,

Annalisa Fasolino

Associate Professor
Institute of Theoretical Physics
University of Nijmegen

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NL-6500 GL Nijmegen

Visiting address:
Toernooiveld 1
Nijmegen

October 18, 2002

Dear Panelist:

I would like to convey my strong support for the work proposed by Professor Shi-Yu Wu and his colleagues on carbon-based quasi one-dimensional nano-structures. My group has been collaborating with Professor Wu's group for a number of years. The two on-going collaborative projects are: (1) Order- N tight-binding molecular dynamics simulations of the mechanical and structural properties of carbon nanorods and (2) electronic transport through carbon-nanotube structures. We are delighted to be working with Dr. Wu's group on these problems.

My group at National Taiwan University has been at the forefront of *ab initio* computational studies of important solid materials such as ultrathin magnetic multilayers, quantum dots and quantum rings as well as carbon nano-structures. In collaboration with Dr. Wu's group, we have recently predicted the possibility of realizing colossal paramagnetic moments for metallic carbon nano-tori [Phys. Rev. Lett. 88, 217206 (2002)]. We have published over 120 refereed papers in the past fifteen years. At the moment, we are especially interested in the development and application of fast linear scaling (order- N) electronic structure methods.

I have visited Louisville at least once a year in the last several years to discuss our collaborative research. Professor Wu has likewise visited National Taiwan University for the same reason. We expect to continue these visits to strengthen our collaborative effort with Dr. Wu's group on the novel mechanical, electronic, and magnetic properties of carbon-based quasi one-dimensional nano-structures.

Yours sincerely,

Guang Yu Guo

Guang-Yu Guo
Professor, Department of Physics
National Taiwan University
Taipei 106, Taiwan
E-mail: gyguo@phys.ntu.edu.tw
Tel: ++886-2-33665180
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LOUISVILLE SCIENCE CENTER

November 8, 2002

Dr. Chakram S. Jayanthi
Department of Physics
University of Louisville
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Executive Director

Dear Dr. Jayanthi:

I would like to express my support for your proposal, "A Comprehensive Study of Carbon-based and Silicon-based quasi-one-dimensional nanostructures: From Fundamental Science to Device Applications" to the DOE/EPSCor. The Louisville Science Center's mission to "improve the public's understanding in science, mathematics and technology through interactive exhibits and programs" directly supports your goal. Being able to develop a new program illustrating nanostructures and their applications would make a significant contribution to our program offerings that bridge science research with the public.

The Science Center has received state and federal funds for exhibit and program development. We have a successful track record of working with university partners through our NIH-SEPA funded program, KY-HEROS. KY-HEROS brings research scientists and their laboratories into the Science Center and throughout Kentucky to work with students, teachers and the general public through exhibit and program offerings. Additionally, the Kentucky Telelinking Network (KTLN) allows the Science Center to offer distance learning programs to over 200 school and university-based sites.

The proposed partnership between the University of Louisville and the Louisville Science Center would build on previous partnerships with the university in engineering, arts and science and health sciences. Our experience disseminating scientific research concepts to a K-12 students and the public, and our capacity to develop effective outreach programs would allow you to reach our broad audience in an engaging and meaningful way.

Developing a new program on nanostructures and technology would help us meet our goals of bringing current research to the public as well as keeping the science center fresh.

I look forward to bringing the Science Center into this exciting research development.

Sincerely,

Gail R. Becker
Executive Director

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Dr. Chakram S Jayanthi
Department of Physics
University of Louisville
Louisville, KY 40292

Dear Dr. Jayanthi:

Please accept this letter as my commitment as educator for the outreach component of your research proposal, "A Comprehensive Study of Carbon-based and Silicon-based quasi-one-dimensional nanostructures: From Fundamental Science to Prototype Devices".

I am pleased to learn of your interest in disseminating your cutting-edge research in nanotechnology to teachers and students in the region. I will serve as an educator and work with your lab and The Louisville Science Center in creating an informative, hands-on educational program. By working with The Louisville Science Center, this program will be accessible to many educators and students throughout the state of Kentucky.

Sincerely,



Nancy Potoczak Miller

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OMB Burden Disclosure Statement

Public reporting burden for this collection of information is estimated to average 15 minutes per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Office of Information Resources Management Policy, Plans, and Oversight, HR-4.3, Paperwork Reduction Project (1910-0400), U.S. Department of Energy, 1000 Independence Avenue, S.W., Washington, DC 20585; and to the Office of Management and Budget (OMB), Paperwork Reduction Project (1910-0400), Washington, DC 20503.

University of Kentucky Research Foundation (Hereinafter called the "Applicant") HEREBY AGREES to comply with Title VI of the Civil Rights Act of 1964 (Pub. L. 88-352), Section 16 of the Federal Energy Administration Act of 1974 (Pub. L. 93-275), Section 401 of the Energy Reorganization Act of 1974 (Pub. L. 93-438), Title IX of the Education Amendments of 1972, as amended, (Pub. L. 92-318, Pub. L. 93-568, and Pub. L. 94-482), Section 504 of the Rehabilitation Act of 1973 (Pub. L. 93-112), the Age Discrimination Act of 1975 (Pub. L. 94-135), Title VIII of the Civil Rights Act of 1968 (Pub. L. 90-284), the Department of Energy Organization Act of 1977 (Pub. L. 95-91), the Energy Conservation and Production Act of 1976, as amended, (Pub. L. 94-385) and Title 10, Code of Federal Regulations, Part 1040. In accordance with the above laws and regulations issued pursuant thereto, the Applicant agrees to assure that no person in the United States shall, on the ground of race, color, national origin, sex, age, or disability, be excluded from participation in, be denied the benefits of, or be otherwise subjected to discrimination under any program or activity in which the Applicant receives Federal assistance from the Department of Energy.

Applicability and Period of Obligation

In the case of any service, financial aid, covered employment, equipment, property, or structure provided, leased, or improved with Federal assistance extended to the Applicant by the Department of Energy, this assurance obligates the Applicant for the period during which Federal assistance is extended. In the case of any transfer of such service, financial aid, equipment, property, or structure, this assurance obligates the transferee for the period during which Federal assistance is extended. If any personal property is so provided, this assurance obligates the Applicant for the period during which it retains ownership or possession of the property. In all other cases, this assurance obligates the Applicant for the period during which the Federal assistance is extended to the Applicant by the Department of Energy.

Employment Practices

Where a primary objective of the Federal assistance is to provide employment or where the Applicant's employment practices affect the delivery of services in programs or activities resulting from Federal assistance extended by the Department, the Applicant agrees not to discriminate on the ground of race, color, national origin, sex, age, or disability, in its employment practices. Such employment practices may include, but are not limited to, recruitment, advertising, hiring, layoff or termination, promotion, demotion, transfer, rates of pay, training and participation in upward mobility programs; or other forms of compensation and use of facilities.

Subrecipient Assurance

The Applicant shall require any individual, organization, or other entity with whom it subcontracts, subgrants, or subleases for the purpose of providing any service, financial aid, equipment, property, or structure to comply with laws and regulations cited above. To this end, the subrecipient shall be required to sign a written assurance form; however, the obligation of both recipient and subrecipient to ensure compliance is not relieved by the collection or submission of written assurance forms.

Data Collection and Access to Records

The Applicant agrees to compile and maintain information pertaining to programs or activities developed as a result of the Applicant's receipt of Federal assistance from the Department of Energy. Such information shall include, but is not limited to the following: (1) the manner in which services are or will be provided and related data necessary for determining whether any persons are or will be denied such services on the basis of prohibited discrimination; (2) the population eligible to be served by race, color, national origin, sex, age, and disability; (3) data regarding covered employment including use or planned use of bilingual public contact employees serving beneficiaries of the program where necessary to permit effective participation by beneficiaries unable to speak or understand English; (4) the location of existing or proposed facilities connected with the program and related information adequate for

determining whether the location has or will have the effect of unnecessarily denying access to any person on the basis of prohibited discrimination; (5) the present or proposed membership by race, color, national origin, sex, age and disability in any planning or advisory body which is an integral part of the program; and (6) any additional written data determined by the Department of Energy to be relevant to the obligation to assure compliance by recipients with laws cited in the first paragraph of this assurance.

The Applicant agrees to submit requested data to the Department of Energy regarding programs and activities developed by the Applicant from the use of Federal assistance funds extended by the Department of Energy. Facilities of the Applicant (including the physical plants, buildings, or other structures) and all records, books, accounts, and other sources of information pertinent to the Applicant's compliance with the civil rights laws shall be made available for inspection during normal business hours on request of an officer or employee of the Department of Energy specifically authorized to make such inspections. Instructions in this regard will be provided by the Director, Office of Civil Rights, U.S. Department of Energy.

This assurance is given in consideration of and for the purpose of obtaining any and all Federal grants, loans, contracts (excluding procurement contracts), property, discounts or other Federal assistance extended after the date hereof, to the Applicants by the Department of Energy, including installment payments on account after such data of application for Federal assistance which are approved before such date. The Applicant recognizes and agrees that such Federal assistance will be extended in reliance upon the representations and agreements made in this assurance, and that the United States shall have the right to seek judicial enforcement of this assurance. This assurance is binding on the Applicant, the successors, transferees, and assignees, as well as the person(s) whose signatures appear below and who are authorized to sign this assurance on behalf of the Applicant.

Applicant Certification

The Applicant certifies that it has complied, or that, within 90 days of the date of the grant, it will comply with all applicable requirements, of 10 C.F.R. 1040.5 (a copy will be furnished to the Applicant upon written request to DOE).

Designated Responsible Employee

John Stencel, Program Director (859) 257-0250

Name and Title (Printed or Typed) and Telephone Number

John Stencel by JKK

Signature and Date

(please type in full name if electronically submitted)

University of Kentucky Research Foundation (859) 257-9420

Applicant's Name and Telephone Number

109 Kinkead Hall; Lexington, KY 40506-0057

Address

12/17/02

Date

Authorized Official:

**President, Chief Executive Officer
or Authorized Designee**

Jack Supplee, Associate Director (859) 257-9420

Name and Title (Printed or Typed) and Telephone Number

Jack Supplee 12/17/02

Signature and Date

(please type in full name if electronically submitted)

CERTIFICATIONS REGARDING LOBBYING; DEBARMENT, SUSPENSION AND OTHER RESPONSIBILITY MATTERS; AND DRUG-FREE WORKPLACE REQUIREMENTS

Applicants should refer to the regulations cited below to determine the certification to which they are required to attest. Applicants should also review the instructions for certification included in the regulations before completing this form. Signature of this form provides for compliance with certification requirements under 10 CFR Part 601 "New Restrictions on Lobbying," and 10 CFR Part 1036 "Governmentwide Debarment and Suspension (Nonprocurement) and Governmentwide Requirements for Drug-Free Workplace (Grants)." The certifications shall be treated as a material representation of fact upon which reliance will be placed when the Department of Energy determines to award the covered transaction, grant, or cooperative agreement.

1. Lobbying

The undersigned certifies, to the best of his or her knowledge and belief, that:

- (1) No Federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure Form to Report Lobbying," in accordance with its instructions.
- (3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers (including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements) and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

2. DEBARMENT, SUSPENSION, AND OTHER RESPONSIBILITY MATTERS

- (1) The prospective primary participant certifies to the best of its knowledge and belief, that it and its principals:
 - (a) Are not presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency;
 - (b) Have not within a three-year period preceding this proposal been convicted of or had a civil judgment rendered against them for commission of fraud or a criminal offense in connection with obtaining, attempting to obtain, or performing a public (Federal, State or local) transaction or contract under a public transaction; violation of Federal or State antitrust statutes or commission of embezzlement, theft, forgery, bribery, falsification or destruction of records, making false statements, or receiving stolen property;
 - (c) Are not presently indicted for or otherwise criminally or civilly charged by a governmental entity (Federal, State or local) with commission of any of the offenses enumerated in paragraph (1)(b) of this certification; and
 - (d) Have not within a three-year period preceding this application/proposal had one or more public transactions (Federal, State or local) terminated for cause or default.
- (2) Where the prospective primary participant is unable to certify to any of the statements in this certification, such prospective participant shall attach an explanation to this proposal.

3. DRUG-FREE WORKPLACE

This certification is required by the Drug-Free Workplace Act of 1988 (Pub.L. 100-690, Title V, Subtitle D) and is implemented through additions to the Debarment and Suspension regulations, published in the Federal Register on January 31, 1989, and May 25, 1990.

ALTERNATE I (GRANTEES OTHER THAN INDIVIDUALS)

- (1) The grantee certifies that it will or will continue to provide a drug-free workplace by:
 - (a) Publishing a statement notifying employees that the unlawful manufacture, distribution, dispensing, possession, or use of a controlled substance is prohibited in the grantee's workplace and specifying the actions that will be taken against employees for violation of such prohibition;
 - (b) Establishing an ongoing drug-free awareness program to inform employees about:
 - (1) The dangers of drug abuse in the workplace;
 - (2) The grantee's policy of maintaining a drug-free workplace;

- (3) Any available drug counseling, rehabilitation, and employee assistance programs; and
- (4) The penalties that may be imposed upon employees for drug abuse violations occurring in the workplace;

(c) Making it a requirement that each employee to be engaged in the performance of the grant be given a copy of the statement required by paragraph (a);

(d) Notifying the employee in the statement required by paragraph (a) that, as a condition of employment under the grant, the employee will:

- (1) Abide by the terms of the statement; and
- (2) Notify the employer in writing of his or her conviction for a violation of a criminal drug statute occurring in the workplace not later than five calendar days after such conviction;

(e) Notifying the agency, in writing, within ten calendar days after receiving notice under subparagraph (d)(2) from an employee or otherwise receiving actual notice of such conviction. Employers of convicted employees must provide notice, including position title, to every grant officer or other designee on whose grant activity the convicted employee was working, unless the Federal agency has designated a central point for the receipt of such notices. Notice shall include the identification number(s) of each affected grant;

(f) Taking one of the following actions, within 30 calendar days of receiving notice under subparagraph (d)(2), with respect to any employee who is so convicted:

- (1) Taking appropriate personnel action against such an employee, up to and including termination, consistent with the requirements of the Rehabilitation Act of 1973, as amended; or
- (2) Requiring such employee to participate satisfactorily in a drug abuse assistance or rehabilitation program approved for such purposes by a Federal, State or local health, law enforcement, or other appropriate agency;

(g) Making a good faith effort to continue to maintain a drug- free workplace through implementation of paragraphs (a),(b),(c),(d),(e), and (f).

(2) The grantee may insert in the space provided below the site(s) for the performance of work done in connection with the specific grant:

Place of Performance: (Street address, city, county, state, zip code)

Center for Applied Energy Research

2540 Research Park Drive

Lexington, Fayette, KY 40511

☒ Check if there are workplaces on file that are not identified here.

ALTERNATE II (GRANTEES WHO ARE INDIVIDUALS)

(1) The grantee certifies that, as a condition of the grant, he or she will not engage in the unlawful manufacture, distribution, dispensing, possession, or use of a controlled substance in conducting any activity with the grant.

(2) If convicted of a criminal drug offense resulting from a violation occurring during the conduct of any grant activity, he or she will report the conviction, in writing, within 10 calendar days of the conviction, to every grant officer or other designee, unless the Federal agency designates a central point for the receipt of such notices. When notice is made to such a central point, it shall include the identification number(s) of each affected grant.

As the duly authorized representative of the applicant, I hereby certify that the applicant will comply with the above certifications.

University of Kentucky Research Foundation, Kentucky DOE EPSCoR Program

NAME OF APPLICANT and PR/AWARD NUMBER and/or PROJECT NAME

Jack Supplee, Associate Director

PRINTED NAME and TITLE OF AUTHORIZED REPRESENTATIVE

Jack Supplee 12/17/02
SIGNATURE and DATE
(please type in full name if electronically submitted)

DEC 18 2002

DEC 18 2002