

Proposal for the development of the

Center for Molecular Design and
Development

at the

University of Arkansas at Little Rock



Department of Chemistry

September 2, 2014

Dr. Joel Anderson, Chancellor
Dr. Zulma Toro Ramos, Provost
University of Arkansas at Little Rock

Dear Drs. Anderson and Toro Ramos:

I am writing this letter to inform you of my request to establish a new center at the University of Arkansas at Little Rock; the *Center for Molecular Design and Development* [CMDD]. I am including numerous documents to support this request. First, I ask you to note the exceptional board of advisors which has been assembled, all of whom have agreed to serve on this center's board. They include:

Dr. Joseph Francisco

William E. Moore Distinguished Professor of
Physical Chemistry, Department of Chemistry,
Purdue University
West Lafayette, Indiana

Dr. Puru Jena

University Distinguished Professor
Department of Physics
Virginia Commonwealth University,
Richmond, VA

Dr. Simon Ang

Director: High Density Electronic Center
Professor of Electrical Engineering
University of Arkansas at Fayetteville, Fayetteville,
Arkansas

Dr. Bobby Sumpter

Deputy Director of the Center for Nanophase
Materials Sciences &
Director for the Nanomaterials Theory Institute
Oak Ridge National Laboratory (ORNL),
Oak Ridge, TN

Dr. Robert O. Shelton

Lead Scientist, Engineering Orbital Dynamics Team
Simulations and Graphics Branch
NASA Johnson Space Center
Houston, TX

Dr. Kenji Yoshigoe

Chair and Associate Professor of Computer Science
Director of NSA Designated Center of Academic
Excellence in Information Assurance &
Director of UALR Computational Research Center
(CRC), University of Arkansas at Little Rock
Little Rock, AR

As you can see, this is an exceptionally outstanding and diverse board which I feel can provide the guidance necessary to make our proposed center one of the best in the country for performing molecular modeling, design and development. I have included a brief biography of each of these board members for your information. In addition, I have provided Letters of Support from numerous individuals (including the proposed board members) who have stated their support for the creation of this center and a commitment of resources from their respective departments or institutions, in order to insure the success of this proposed center. These include letters from: **Dr. Joseph Francisco**, William E. Moore Distinguished Professor of Physical Chemistry, Purdue University; **Dr. Puru Jena**, Distinguished Professor, Virginia Commonwealth University; **Dr. Robert Shelton**, NASA Johnson Space Center;

Dr. Simon Ang, Director, High Density Electronic Center, Fayetteville AR; **Dr. Bobby Sumpter**, Deputy Director, Oak Ridge National Lab; **Dr. Kenji Yoshigoe**, Chair and Director of UALR Computational Research Center; **Dr. Keith Hudson**, Director GIT, UALR; **Dr. John Bush**, Chair, Department of Biology, UALR; **Dr. Jeff Gaffney**, Chair, Department of Chemistry, UALR; **Dr. Elizabeth Pierce**, Chair, Department of Information Science, UALR; **Dr. Antonie H. Rice**, Chair, Department of Chemistry & Physics, UAPB; **Dr. Parthasarathy Tigulla**, Distinguished Professor, Osmania University, Hyderabad, India. Dr. Tigulla is of particular significance because of his interest in establishing an exchange program for both faculty and students between UALR and Osmania University in India. I should point out that Osmania University is one of the largest university systems on the subcontinent of India with over 300,000 students on its campuses and affiliated colleges. Dr. Tigulla is particularly interested in a collaborative venture involving bioinformatics and computational modeling. We have also discussed joint funding ventures in which he has stated that there is considerable financial support for inter-institutional collaborations from his university and from the Indian government. I should also mention that NIH and NSF have programs to fund international collaborative efforts. Dr. Tigulla has agreed to participate in all such funding programs and exchanges.

In summary, as can be seen from the considerable number of Letters of Support, there is significant support within the College of Arts, Science and Letters and the College of Engineering and Information Technology (EIT) at UALR. In addition, there is considerable support from other institutions within the state of Arkansas such as the University of Arkansas, Fayetteville and the University of Arkansas at Pine Bluff as well as national and international support from scientist and/or faculty at NASA's Johnson Space Center, Oak Ridge National Labs, Virginal Commonwealth University, Purdue University and Osmania University in Hyderabad, India. As a result of this diverse support, I can see no downside and can see only upside to developing this center on the UALR campus. As stated in several support letters, this center will be unique in the state of Arkansas and will provide a valuable resource for this state. The nearest center similar to the one being proposed is located at Texas A&M University in College Station, Texas. I anticipate the main source of funding for the center will be from externally funded grants and foundations. I hope I can count on the UALR administration's support for this new proposed center. If you have any further questions, please do not hesitate to contact me.

Thank you very much,



Jerry A. Darsey, PhD
Professor of Chemistry

LETTER OF NOTIFICATION

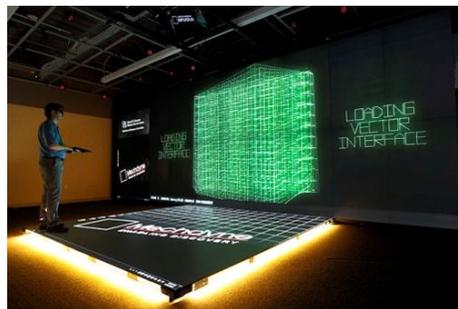
ESTABLISHMENT OF NEW CENTER UNIT

(Center, Division, or Institute not offering primary faculty appointments, or certificate or degree programs)

1. **Institution submitting request:** University of Arkansas at Little Rock (UALR)
2. **Contact person/title:** Jerry A. Darsey, Professor, Department of Chemistry, University of Arkansas at Little Rock
3. **Mailing Address:** Department of Chemistry, University of Arkansas at Little Rock, Little Rock, AR 72204
4. **Phone number/e-mail address:** (501) 569-8828 / jadarsey@ualr.edu
5. **Name of Proposed Administrative Unit:** Center for Molecular Design and Development [CMDD]
6. **Proposed Location:** Science Laboratory Building (SCLB), Rooms 452/485, UALR
7. **Distance of proposed unit from main campus:** 0 mile
8. **Reason for proposed action:** The Center for Molecular Design and Development [CMDD] will be using the most powerful molecular modeling procedures, for solving complex computational problems involving molecular systems. This center will be used for simulation, data mining, and visualization to solve various molecular simulation problems which are not possible by other theoretical or experimental approaches. Unlike physical experimentation, modeling and simulation is cost effective, safe, and flexible. Furthermore, CMDD uses tools which can model and evaluate problems which have not had any evaluation or simulation attempted on it thus far. There will be a heavy emphasis on drug design and development. CMDD represents, in many ways, the most effective mechanisms for approaching advanced molecular discoveries using the most powerful state-of-the-art methods for their design and development. This will enhance discoveries and developments in the areas of drug design, new nanomaterials (such as new solar cells, fuel cells, biomaterials), new polymeric materials, catalytic materials, etc. with a high probability for patentability.

The Center for Molecular Design and Development will utilize the high performance computing (HPC) and visualization facilities available in the Donaghey College of Engineering and Information Technology (EIT), as well as capabilities at Oak Ridge National Labs, NASA, Virginia Commonwealth University, University of Arkansas, Fayetteville and Purdue University. At UALR, there has been a steady growth in terms of infrastructure as well as service capabilities for the past several years. This includes the newest visualization capabilities at the George W. Donaghey Emerging Analytics Center (EAC).

This center is a partnership between Mechdyne Corporation and UALR. Mechdyne's installation at UALR is the world's first EmergiFLEX™ immersive visualization technology. The ability to easily move the EmergiFLEX's wall screens in the EAC Virtual Data Lab make this ideal for applications that will benefit from more than one display configuration, as seen in the figure above. The display



environment consists of three walls and one floor screen. The side walls can be moved independently to create new formats. In less than a few minutes the EmergiFLEX™ can become:

- A flat wall display for presentation or data review
 - An angled theatre, perfect for team collaboration or to display multiple datasets on different screens
 - An L-shape for combined immersive mode and data display
 - A CAVE-like immersive room for 3-D spatial structures
- The side screens can be moved by a single person and feature Mechdyne's exclusive self-leveling side screens and Integrated Structural System eliminating alignment adjustments after reconfiguration.

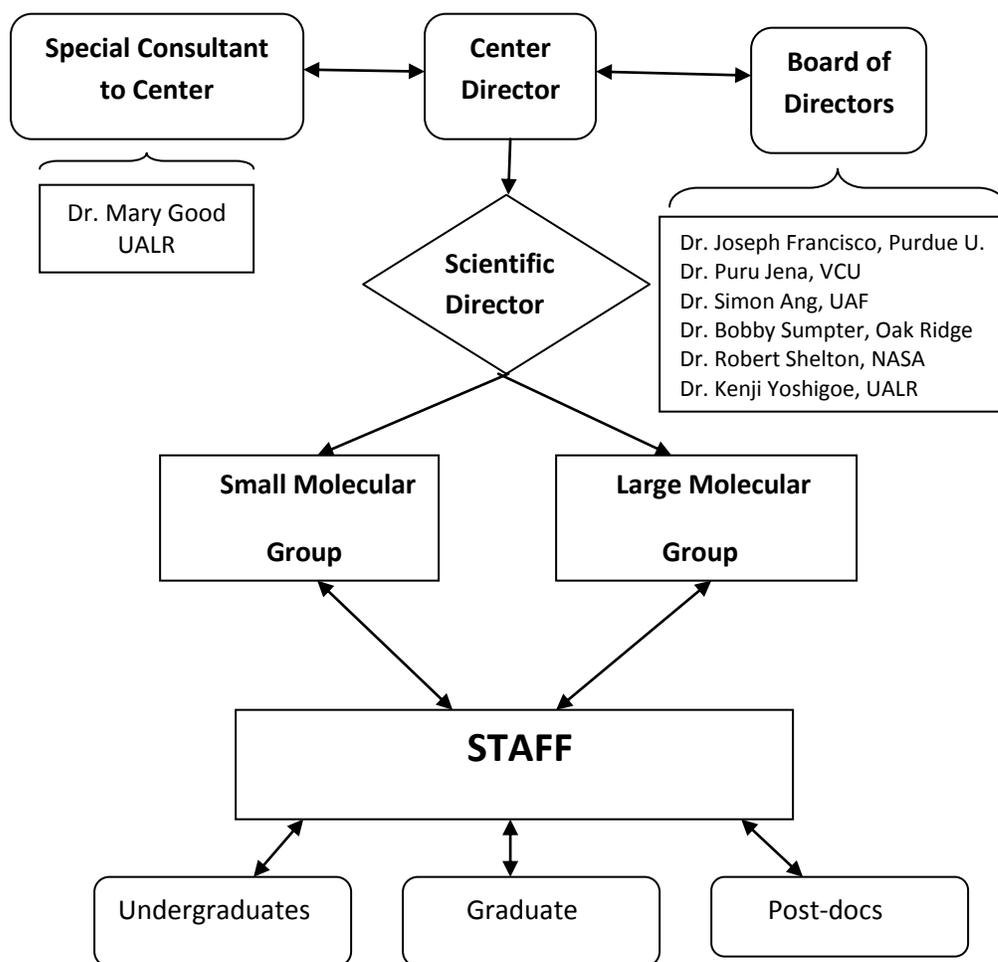
Since HPC's first deployment, it serves a critical role in various research projects at UALR and its collaborators. Faculty and student researchers of EIT, the College of Arts, Science and Letters and researchers of the University of Arkansas for Medical Sciences (UAMS) will be major collaborators at the center, and this collaboration is expected to grow. The facility needs to become an administrative unit at UALR in order to:

- a. Excel in, and improve upon, research productivity at the UALR, and the other participating institutions. The center will utilize the current and future visualization and HPC resources, and use of these facilities, will allow researchers in various disciplines, from inside as well as outside the science and engineering community, to advance knowledge at a pace which has not been possible in traditional theoretical and modeling approaches.
 - b. Provide technical and infrastructural resources to Arkansas and participating organizations. Using our most advanced visualization and HPC capabilities to accelerate modeling and simulation of molecular systems, in order to provide a significant competitive advantage when applying for grants to both federal agencies such as NSF, DoE, DoD, NIH, etc. as well as private agencies such as the Michael J. Fox Foundation and the Melissa and Bill Gates Foundation, etc.
 - c. Enhanced ability to obtain and sustain financial support which can provide the necessary support for the center and the students and staff working in the center—The CMDD center will provide valuable support to researchers within UALR and outside. Once the Center for Molecular Design and Development is established, the directors of the center will mount a sustained marketing effort to widen the visibility of the center for its sustained viability, which will highlight its capabilities and promote it as one of the top molecular simulation and modeling centers in the country.
9. Mission and role for proposed unit: The mission of the Center for Molecular Design and Development (CMDD) is to improve our abilities to use state-of-the-art modeling to provide predictive algorithms for creating new molecular systems with desired characteristics. Such algorithms could be used to solve problems ranging from biochemical to materials science applications. This will be accomplished by CMDD by bringing together the expertise, capabilities, and resources necessary for solving predictive modeling problems. This includes the necessary hardware, software, and human resources needed to accomplish this goal. The CMDD will provide a platform for the enhanced education of students at the undergraduate and advanced levels of education. CMDD will also be a multi-university facility with a number of in-state and out-of-state institutions and will function as a national resource. This center is designed to contribute as a major research facility for the University of Arkansas at Little Rock and the state of Arkansas. The center will function to:

- a. Acquire hardware and software resources to accommodate current and future computing requirements;
- b. Manage and optimize the use of computing and storage resources;
- c. Provide modeling expertise to maximize existing computing and data storage capabilities;
- d. Assist users in the execution of modeling software applications;
- e. Guide migration of user jobs to XSEDE (eXtreme Science and Engineering Discovery Environment) and other large-scale computing, visualization, and storage systems;
- f. Help to maintain computing and data storage systems purchased by CMDD for use by individual faculty members;
- g. Promote value of computational and modeling research at the University of Arkansas at Little Rock;
- h. Establish and sustain collaborative activities with other HPC and related organizations;
- i. Provide resources and expertise to other Arkansas institutions such as the University of Arkansas, Fayetteville, the University of Arkansas at Pine Bluff, the University of Arkansas for Medical Sciences, Arkansas State University, and any other Arkansas institution which would find the capabilities of CMDD a valuable resource;
- j. Use Informatics and Quantum Mechanical Modeling for identifying new drug molecules for the treatment of numerous diseases, such as Parkinson's Disease, Tuberculosis, Multiple Sclerosis, Alzheimer's, Myeloproliferative disease, and many more.

Organizational Chart

Center Organization



Center for Molecular Design and Development

Board Members

Center for Molecular Design and Development [CMDD]

Advisory Board



Dr. Joseph Francisco
William E. Moore Distinguished Professor of Physical
Chemistry
Department of Chemistry
Purdue University
West Lafayette, Indiana



Dr. Puru Jena
University Distinguished Professor
Department of Physics
Virginia Commonwealth University,
Richmond, VA



Dr. Simon Ang
Director: High Density Electronic Center
Professor of Electrical Engineering
University of Arkansas at Fayetteville, Fayetteville, AR



Dr. Bobby Sumpter
Deputy Director of the Center for Nanophase Materials
Sciences &
Director for the Nanomaterials Theory Institute
Oak Ridge National Laboratory (ORNL),
Oak Ridge, TN



Dr. Robert O. Shelton
Lead Scientist, Engineering Orbital Dynamics & SIM Team
Simulations and Graphics Branch
NASA Johnson Space Center
Houston, TX



Dr. Kenji Yoshigoe
Chair and Associate Professor of Computer Science
Director of NSA Designated Center of Academic
Excellence in Information Assurance &
Director of UALR Computational Research Center (CRC)
University of Arkansas at Little Rock

Center for Molecular Design and Development

Biographies

Board Members

Biography

Dr. Joseph S. Francisco

William E. Moore Distinguished Professor of
Physical Chemistry
Department of Chemistry
Purdue University
West Lafayette, Indiana



Joseph S. Francisco was President of the American Chemical Society from 2009-2010. He currently serves as the William E. Moore Distinguished Professor of Physical Chemistry, and, Earth and Atmospheric Sciences at Purdue University in West Lafayette, Indiana. He received his bachelors degree from the University of Texas at Austin in 1977 and his PhD from the Massachusetts Institute of Technology in 1983. He was President of the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers from 2006–2008. He is also a fellow of the American Physical Society, the American Association for the Advancement of Science, American Chemical Society, and a Guggenheim Fellow. He was awarded an Alexander von Humboldt U.S. Senior Scientist Award, appointed a Senior Visiting Fellow at the Institute of Advanced Studies at the University of Bologna, Italy; Professeur Invité at the Université de Paris-Est, France; a Visiting Professor at Uppsala Universitet, Sweden; and an Honorary International Chair Professor, National Taipei University of Technology, Taiwan. He was elected as the Fellow of the American Academy of Arts and Sciences in 2010 and was elected member of the U.S. National Academy of Sciences in 2013. He also received Honorary Doctor of Science Degrees from Tuskegee University in 2010 and the University of Arkansas at Little Rock in 2011. He was appointed to serve on the President's Committee on the National Medal of Science for the period 2010–2012 and 2012–2014.

Research in Dr. Francisco's laboratory focuses on basic studies in spectroscopy, kinetics and photochemistry of novel transient species in the gas phase. These species play an important role in atmospheric, biochemical and combustion processes. Yet questions dealing with how structures correlate to reactivity and photochemical mechanisms have not been addressed for these systems. These problems are addressed by research efforts in our laboratory. Specific research areas of interest are: 1) Spectroscopic determinations of electronic and vibrational transitions in free radicals; 2) Measurement of the kinetics of individual gas-phase reaction steps involving free radicals in complex reaction mechanisms; and 3) Characteristics of primary photo chemical processes that free radicals can undergo.

Theoretical and experimental methods are used cooperatively in extending spectroscopic information on these species. Our goal is to use state-of-the-art molecular orbital methods to predict the properties that can be used as a guide in the experimental search. Using a variety of high resolution laser techniques, such as laser-induced fluorescence, vibrational and electronic emission, multi-photon and UV absorption spectroscopy, we aim to make spectroscopic measurements for these novel species in the gas phase, and fully characterize them. Dr. Francisco has published more than 400 journal articles, written nine book chapters, co-authored the textbook *Chemical Kinetics and Dynamics*, and served on numerous national science councils.

Joseph Francisco has most recently been appointed as the Dean of the College of Arts and Sciences at The University of Nebraska-Lincoln. Ellen Weissinger, senior vice chancellor of academic affairs announced this appointment of Dr. Francisco as dean of the university's largest college. "As a researcher and an educator, Joe has demonstrated the highest level of performance at every stage of his career and he has a rare talent for inspiring excellence in others," Weissinger said. Dr. Francisco will begin his new duties on July, 1, 2014.

Biography

Dr. Puru Jena

University Distinguished Professor
Department of Physics
Virginia Commonwealth University,
Richmond, VA



Dr. Purusottam (Puru) Jena, Distinguished Professor of Physics at Virginia Commonwealth University received B. Sc. (Hons) and M. Sc. in Physics from Utkal University, India and Ph. D. in Physics from the University of California at Riverside. After postdoctoral and visiting appointments at State University of New York, Albany; Dalhousie University, Halifax, Canada, University of British Columbia, Vancouver, Canada, Northwestern University, Evanston, and Argonne National Laboratory he joined the Physics faculty of Michigan Technological University, Houghton. He moved to Virginia Commonwealth University, Richmond in 1980 where he has remained ever since with the exception of a year (1986-87) as a Program Director at the Materials Science Division of the National Science Foundation, and a year (2007-08) as a Jefferson Science Fellow and Senior Science Advisor at the US Department of State.

Dr. Jena's research covers a wide range of topics in condensed matter, atomic, and molecular Physics. These include electronic structure of metals, semiconductors, superconductors, alloys, liquid metals, point and complex defects, surfaces, thin films, atomic clusters, cluster assembled materials, nanoscience, and nanotechnology. His current research involves three major areas: structure and properties of nanoclusters and cluster assembled materials, renewable energy with particular emphasis on hydrogen storage, and spintronics. Dr. Jena is the author of nearly 450 papers including editor of 12 conference proceedings. He has given over 350 invited talks in international conferences and academic institutions in nearly 30 countries around the world.

Dr. Jena's honors include: Jefferson Science Fellow at the US Department of State, David Hare Professorship lecture at the Indian Association for Cultivation of Science, Kolkata, India; Fellow of the American Physical Society, Outstanding Faculty Award from the State Council of Higher Education of Virginia; University Award of Excellence and Outstanding Scholar Award from Virginia Commonwealth University; and Chair of the Gordon Conference on Metal-Hydrogen Interactions. He has organized more than thirty international conferences and has served as a member of scientific panels for the National Science Foundation, Department of Energy, and Army research Office. He was a member of the Executive Committee that drafted the report on the "Basic Research Needs for the Hydrogen Economy" for the Department of Energy. He has also served on the Virginia Governor's task force on green energy technologies.

Biography

Dr. Simon Ang

Director: High Density Electronic Center
Professor of Electrical Engineering
University of Arkansas at Fayetteville,
Fayetteville, AR



Simon Ang graduated with a B.S. Degree in Electrical Engineering from the University of Arkansas at Fayetteville. He subsequently completed the M.S. Degree in Electrical Engineering at Georgia Institute of Technology, Atlanta, Georgia, and the Ph.D. Degree in Electrical Engineering at Southern Methodist University, Dallas, Texas. Dr. Ang worked for seven years at Texas Instruments Inc., in Dallas, Texas, holding a variety of increasingly responsible positions, including a section manager in the Advanced Power Integrated Circuit Development Center prior to joining University of Arkansas. He is now a full Professor of Electrical Engineering.

Simon has received numerous teaching awards, including the Arkansas Alumni Association Distinguished Achievement Award in Teaching in 1994. He has supervised over 110 M.S. and Ph.D. students in electrical engineering, biomedical engineering, mechanical engineering, and agricultural engineering. He received the Insignia Award in Technology from the City and Guilds of London Institute, England in 1988 for his work on power semiconductor device development. He is the author and/or co-author of more than 260 journal and proceeding articles and six book chapters. He holds four U.S. patents. He is the author of the book "Power Switching Converters" (Marcel Dekker, 1995), the principal author of "Power-Switching Converters -2nd Edition" (CRC Press, 2005), and "Power-Switching Converters - 3rd Edition" • (CRC Press 2010).

Simon is a licensed professional engineer and has acted as a technical advisor and consultant to a number of industrial clients. Simon's fields of research include microelectronics and power electronics packaging, high-density and high-temperature power electronic systems, mixed signal circuit design and test, biomedical and electrical instrumentation, sensors, micro-electromechanical systems, power management circuits and systems, LED systems, power semiconductor devices, photovoltaic electronics, and switching converters. Simon was involved in the initial formation of HiDEC in 1992 and served one term as its Co-Director from 1998-2001. He is a visiting Professor at Nanyang Technological University, Singapore. Dr. Ang is a Fellow of the Institute of Electrical and Electronics Engineers (IEEE), Institution of Engineering and Technology (IET-UK), City and Guilds of London Institute (UK), and the Electrochemical Society.

Biography

Bobby G. Sumpter

Deputy Director of the Center for
Nanophase Materials Sciences &
Director for the Nanomaterials Theory
Institute
Oak Ridge National Laboratory(ORNL),
Oak Ridge, TN



Education, Professional Experience, Activities, and Honors: Bobby

G. Sumpter received his Bachelor of Science in Chemistry from Southwestern Oklahoma State University(1983) with minors in Mathematics, Physics, Computer Science, and Geology. He received a Ph.D. in Physical Chemistry from Oklahoma State University in 1986. Following postdoctoral studies in Chemical Physics at Cornell University 1987-1988 and in Polymer Chemistry at the University of Tennessee. Bobby joined the Chemistry Division at Oak Ridge National Laboratory in the Polymer Science group in 1992. He serves as an Advisory Committee Member of the "International Journal of Smart Engineering System Design" and on the editorial board of "Research Letters in Nanotechnology". He is a continuing co-organizer of the annual international meeting, Artificial Neural Networks in Engineering, Co-organized and Chaired the 1st DOE Workshop on Applications of Neural Networks in Materials Science (Feb 28-March 2, 1994), Co-organized a symposium at the 1999 SERMACS meeting, and Co-organized and chaired the modeling and simulation track at the IEEE NANO 2008 meeting. Bobby has authored or co-authored over 300 publications in refereed journals. He is a member of the American Chemical Society, American Association for the Advancement of Science, , American Physical Society, American Institute of Chemists, Sigma XI, International Neural Network Society, Materials Research Society. Bobby was part of a research team that received the ORNL-CASD Technical Achievement Award in 1996 and the Lockheed Martin Energy Research significant advent award 1999.

Interests and Expertise: Dr. Sumpters' research interests are focused on understanding the chemistry and physics of molecular systems with emphasis at the nanoscale level. Particular focus is on theoretical and computational study of: chemistry in nano-confined environments, nanoscale self assembly and self organization processes, fundamental structure and dynamics of molecular-based materials including multi-component polymers and nano-composites, elucidation of the physical, mechanical and electronic properties of nanoscale materials, advanced quantum chemistry, and biotechnology.

Biography

Dr. Robert O. Shelton

Lead Scientist, Engineering Orbital Dynamics & SIM Team
Simulations and Graphics Branch
NASA Johnson Space Center
Houston, TX



Dr. Robert Shelton is currently manager, Technology Branch of the Education Office at the Johnson Space Center (JSC). He received his Ph.D. in Mathematics from Rice University in 1975, and received BA in Mathematics from Rice University in 1971. He worked as Postdoctoral Fellow at Institute for Advanced Studies, Princeton, N.J. Dr. Shelton is responsible for the Digital Learning Network and Web Applications group at NASA Johnson Space Center. He is also Lead Scientist for the Engineering Orbital Dynamics & SIM Team Simulations and Graphics Branch at NASA Johnson Space Center.

His research interest include designing intelligent systems such as neural networks, designing and developing innovative interface software to represent data in a form accessible to students with vision or perception disabilities. He developed Math Description Engine (MDE) to provide alternative accessibility for students with vision or perception disabilities. MDE uses rule-based and computational machine intelligence, feature extraction, and description synthesis to analyze, describe and signify equations and data. He developed an Artificial Intelligence software program involving artificial neural networks, NETS; a tool for the development and evaluation of neural networks, and provides a simulation algorithm plus an environment for developing such algorithms.

Dr. Shelton received many exceptional awards for outstanding research. He received Laureate for The Tech Museum Award - Technology Benefiting Humanity, for the year 2007. He received NASA Software runner-up award for the year 2006, for his software on Artificial Neural Networks, received NASA Exceptional Service Medal for 2001, and received National Business & Disability Council Award of Honor. Johnson's Space Center honored him with JSC Director's Innovation Award for the year 2004. Dr. Shelton is the author of almost 100 publications, and received 2 patents. With his exceptional performance, he received many accolades from research community at the Johnson Space Center.

Dr. Shelton, developed software tools for students, researchers and educators. Products included ILIAD (1995), an intelligent meta-search agent for teachers; NASA Qwhiz (1998), an interactive, multi-player, web-based science challenge game; ROVer Ranch(2000), an interactive web-based robotic lab with 3-d VRML simulation environment.

Biography

Dr. Kenji Yoshigoe

Chair and Associate Professor of Computer Science

Director of NSA Designated Center of Academic Excellence in Information Assurance &

Director of UALR Computational Research Center (CRC)

University of Arkansas at Little Rock



Dr. Kenji Yoshigoe, is associate professor of Computer Science at the University of Arkansas at Little Rock (UALR). He received a Ph.D. in Computer Science and Engineering from University of South Florida in 2004. He received his B.S. in Computer Science from University of South Florida in 2000. His research explores new algorithms, protocols, and architectures for scalable computing and communication systems. He is currently investigating the scalability, reliability, and security of systems ranging from high performance computing systems to wireless sensor networks.

Currently, Dr. Yoshigoe is working as Chair of the Department of Computer Science at UALR, is a founding Director of UALR's Computational Research Center (CRC), and a founding Director of the NSA Designated Center of Academic Excellence in Information Assurance. CRC is dedicated to the promotion of efficiency, productivity, and accuracy in research through the use of significant and diverse computing resources and is designed in such a way to address the diversity of research community and to serve varied computational requirements of this diversified environment at UALR. This center is unique to Arkansas and brings a new level of computing capacity and capability to education, corporate, and government research organizations.

Dr. Yoshigoe is the author of nearly 150 publications, and 40 conference proceedings. He served as dissertation advisor for many Ph.D. students in Computer Science department, and served as a committee member for many additional doctoral students. He is an editorial board member of IET Wireless Sensor Systems, and River Publishers Journal of Cyber Security and Mobility - Special Issue on Big Data Theory and Practice. He is an advisory board member of Critical Task Site Selection, Information Technology Training Center (ITTC) at the National Guard Professional Education Center. Dr. Yoshigoe is also on the program committee of IEEE Global Wireless Summit, the International Symposium on Modeling and Optimization, and IEEE International High Assurance Systems Engineering.

Special Consultant to the Center

Biography:**Dr. Mary L. Good**

Dean Emeritus and Founding Dean
Donaghey College of Engineering and
Information Technology
University of Arkansas at Little Rock



Mary Lowe Good is an inorganic chemist who has performed industrial research and has worked in government. She received her BS from the University of Central Arkansas and in 1955 received her PhD in from the University of Arkansas in Fayetteville. In 1980 she was appointed to the National Science Board of the National Science Foundation by Jimmy Carter and then in 1986 she was appointed to it again by Ronald Reagan. In 1976 she was initiated into the Beta Phi Chapter of Alpha Chi Sigma at the South Dakota School of Mines.

Former President Bush appointed her to the President's Council of Advisors on Science and Technology (PCAST). Later Dr. Good in 1993 served four years as the Under Secretary for Technology for the Technology Administration in the Department of Commerce, under the Clinton Administration.

She was the 1987 President of the American Chemical Society.

She has also been a Donaghey University Professor at the University of Arkansas at Little Rock, and was the founding Dean of the George W. Donaghey College of Engineering and Information Technology (EIT), retiring July 1, 2011.

She has been member for Fund for Arkansas, LLC and Stage 1 Diagnostics, and has served on the boards of Delta Trust & Bank and St. Vincent Infirmary, Biogen Idec, IDEXX Laboratories, Cincinnati Milacron, Ameritech, Acxiom Corporation.

Mary L. Good is a highly regarded chemist whose multifaceted career has ranged from academia, to the industrial sector, to the national government, where she serves as undersecretary of technology in the Department of Commerce. Good is described by Jeffrey Trehitt in *Chemical Week* as an unabashed proponent of industrial chemistry. She told Trehitt that "we've ... gotten ourselves into a trap.... The word 'chemical' has become a bad name, and yet, without chemicals the world doesn't move. We've got to develop a better perspective." She is also a managing member of the Fund for Arkansas' Future, an organization that aims to foster high-tech business and industry in Arkansas. In addition to chemistry, she enjoys fly-fishing and Scottish history.

Center for Molecular Design and Development

Letters of Support

June 9, 2014

Dr. Joel Anderson, Chancellor
University of Arkansas at Little Rock
Little Rock, AR 72204

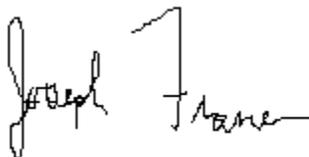
Dear Chancellor Anderson:

I am writing this letter to strongly support Dr. Jerry Darsey's proposed development of the Center for Molecular Design and Development. I believe that such a center would greatly facilitate and encourage interactions between faculties at universities within the state of Arkansas. It should also facilitate interdisciplinary collaborations between faculty members within UALR and between faculty members at other universities.

I believe this center would be the only center of its kind in Arkansas and among the few centers of its kind in the mid-south. In my lab, we incorporate theoretical methods in modeling and predicting spectroscopic information of various molecular species. I can visualize a symbiosis between much of the work we perform at my lab and the proposed center at UALR with its proposed theoretical modeling capabilities. The type of center being proposed will provide the capabilities to model all of the variety of systems we study in my research. I can certainly envision a strong collaborative interaction between my lab at and UALR.

In addition, this center can be a valuable asset for any researcher whose goal is to use the latest state-of-the-art molecular orbital methods. This could extend to developing molecular species ranging from new catalytic molecules to potentially new drug molecules. In summary, I strongly support the creation of the Center for Molecular Design and Development at the University of Arkansas at Little Rock. Given the potential implications of the products and services which can come from this center, and the need for one like this in the state of Arkansas, I can only see very positive benefits to UALR and the State of Arkansas. I would like to fully offer my cooperation and support for the formation of this center and am honored to be invited to serve on its Board of Advisors.

Sincerely,



Joseph S. Francisco,
William E. Moore Distinguished Professor of Physical Chemistry

April 28, 2014

To Whom It May Concern:

It is my pleasure to recommend the efforts of Dr. Jerry Darsey to create the Center for Molecular Design and Development on the campus of the University of Arkansas at Little Rock. From the information I was provided, there is no center in Arkansas that has the goals or capabilities of this proposed center. Molecular modeling has become one of the most powerful tools available to scientist for determining properties of various molecular systems. Dr. Darsey and his group have been at the forefront of many of these modeling procedures. One particular modeling method which Dr. Darsey and his group helped pioneer is the use of various artificial intelligence (AI) procedures to predict the physical and chemical properties of molecules.

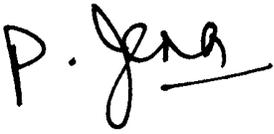
One particular area where the method of using AI procedures was applied was in one of Professor Darsey's PhD students who recently graduated. I was on this students PhD committee so I am familiar with the research. This student used AI methods for two very diverse applications. The first use was in the analysis of genetic information on Tuberculosis patients. He was able to find genetic markers within this data to correlate genetics with the susceptibility to contract TB. In fact, he was able to model this genetic data to find which particular type of TB the patient was most susceptible to.

A second part of this student's dissertation was in the modeling of materials for use in the storage of hydrogen gas for use in a potential future hydrogen economy. Hydrogen is one of the most environmentally neutral fuel sources available. Its byproduct is water vapor. One of the greatest obstacles to developing hydrogen as a fuel is storage. Currently there are only two methods to store sufficient hydrogen for applications. One is in tanks at high pressure, up to 10,000 psi. The other is at cryogenic temperatures. Dr. Darsey's student was able to model metallic hydride nanomaterials for potential use in storage of large amounts of hydrogen in a relatively small volume at normal room temperatures. The procedure used for this modeling was artificial intelligence.

As a person who has personally known Dr. Darsey for many years and one who knows of the more than 100+ publications, a recent book on the subject of AI molecular modeling and invitations to organize and chair many national and international conferences, I know of no one more qualified to develop a center devoted to the modeling of molecular systems. I give his request my highest recommendation.

If you have any questions, please do not hesitate to contact me.

Sincerely,

A handwritten signature in black ink that reads "P. Jena". The signature is written in a cursive style with a horizontal line extending from the end of the name.

Puru Jena
Distinguished Professor of Physics



UNIVERSITY OF ARKANSAS

— THE YOU OF A —

3217 Bell Engineering Center • Fayetteville, Arkansas 72701 • (479) 575-3005 • (479) 575-7967 (FAX)
College of Engineering
High Density Electronics Center

April 25, 2014

Jerry A. Darsey, Professor
Chemistry Department
University of Arkansas at Little Rock
Little Rock, AR 72204

Dear Dr. Darsey:

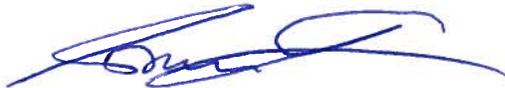
It is my great honor to support your efforts to establish on your campus, the Center for Molecular Design and Development (CMDD). This center would be a valuable asset for the University of Arkansas at Little Rock as well as the University of Arkansas, Fayetteville. As the Director of the High Density Electronics Center, I am very much in need of computational capabilities to model many of the systems we study at our center. As such, I asked Dr. Darsey to join our effort to secure a grant from the Department of Energy for \$4.7 million. It is my strong belief that without the modeling capability of Dr. Darsey's group, the proposal to DoE would not be nearly as strong.

The exact computational effort of Dr. Darsey's group relates to performing modeling studies on catalytic materials for use in the development of Proton Exchange Membrane (PEM) fuel cells. I am very confident that Dr. Darsey's group can shed some fundamental insight on some of the catalytic materials which can take the place of platinum (Pt) as a material for PEM fuel cells. The major problem with Pt catalyst is that it is very expensive. It will be absolutely necessary to find substitute catalytic materials before a truly commercial fuel cell can be developed. His group has been at the forefront of molecular modeling of such materials. I am also aware of several other groups which have collaborations with Dr. Darsey's group. These collaborations have resulted in numerous presentations at national meetings as well as numerous publications.

Another area where I am familiar with Dr. Darsey's modeling is in the area of predicting materials capable of storing large quantities of hydrogen gas. Before a viable fuel cell energy capability can be realized, there must be a way of storing hydrogen, the fuel necessary for many fuel cell systems. Current methods for storing hydrogen gas would not be very practical or safe. The current method for storing enough hydrogen for use in transportation applications, such as automobiles, trucks, etc., is in the form of gas stored in cylinders at very high pressures (10,000+ psi) or at cryogenic temperatures (-270 °C). Neither of these current methods would be practical. Dr. Darsey has studied materials such as metal hydrides and metal organic frameworks, which have demonstrated the capability of storing a larger volume of hydrogen gas at room temperature without the dangers of high pressure or cryogenic temperatures.

Therefore it is with my unqualified support that the Center for Molecular Design and Development be established at UALR and I will support this center with the resources available at our High Density Electronics Center at Fayetteville. Please feel free to contact me if you have any questions.

Sincerely,



Simon S. Ang, PhD, PE, FIEEE, FECS, FIET(UK), FCGI(UK)
Director, High Density Electronics Center
Professor of Electrical Engineering

OAK RIDGE NATIONAL LABORATORY

MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

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May 1, 2014

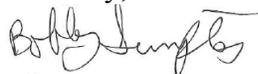
Dr. Jerry A. Darsey
Department of Chemistry
University of Arkansas at Little Rock (UALR)

Re: Letter of Support

Dear Dr. Darsey,

I am writing this letter to express my support of the proposed new center, "Center for Molecular Design and Development [CMDD]". Many aspects of this center, such as using the most powerful molecular modeling procedures for solving complex computational problems involving molecular systems, are closely aligned with the scope of some of our activities at the Center for Nanophase Materials Sciences (CNMS), a scientific user facility supported by the U.S. Department of Energy, Basic Energy Sciences. Based on the importance of your proposed center and the outstanding reputation of your team, I am confident that we can work together on various projects (facilitated through approved CNMS user projects) and I am honored to serve on the advisory committee for the CMDD. I also believe the efforts of your proposed center would further strengthen and sustain existing collaborations and that it would particularly benefit student training and educational efforts, which in turn could further strengthen student recruiting and retention for projects in STEM fields.

Sincerely,



Bobby G. Sumpter
Director, Nanomaterials Theory Institute, Center for Nanophase Materials Sciences
Group Leader, Computational Chemical and Materials Sciences, Computer Science &
Mathematics Division
Oak Ridge National Laboratory, Oak Ridge TN 37831-6494

cc Hans Christen

National Aeronautics and
Space Administration

Lyndon B. Johnson Space Center
2101 NASA Parkway
Houston, Texas 77058-3696



May 16, 2014

Reply to Attn of: ER-14-022

Jerry A. Darsey, Professor
Department of Chemistry
University of Arkansas at Little Rock
Little Rock, AR 72204

Professor Darsey I am writing to express my enthusiastic support for the proposed Center for Molecular Design and Development (CMDD). The CMDD will bring together a diverse collection of talent from chemistry, materials science, physics, mathematics and computer science to explore and develop means of identifying and synthesizing new materials based on their molecular properties. Your previous work which pioneered the use of advanced pattern recognition algorithms in connection with molecular dynamics and quantum mechanical models to predict macroscopic properties of new substances is a harbinger of the sort of breakthroughs which could be enabled by the CMDD. The power of this approach lies in the ability to scan vast numbers of molecular configurations for those rare combinations which are predicted to exhibit desirable macroscopic properties. The ability to simulate and predict enables consideration of vastly more possibilities than would be possible by conventional means.

The people involved have a significant history of useful collaboration. Although most of my publications are in pure mathematics or machine learning, Professor Darsey and I have published joint work which benefitted from the diverse experience of all the authors. The center will not only attract a critical mass of people who have a history of collaboration on related projects in the past, but also will provide a structure for exchange of ideas which is essential for research which spans so many diverse disciplines. I strongly support this proposal and look forward to a vigorous collaboration enabled by the center.

A handwritten signature in black ink, appearing to read "Robert Shelton".

Dr. Robert Shelton
Lead, JSC Engineering Orbital Dynamics and Morpheus Sim Team
Simulation and Graphics Branch
NASA Lyndon B. Johnson Space Center
2101 NASA Parkway
Houston, TX. 77058

April 22, 2014

To Whom It May Concern:

It is my great pleasure to express my support for the establishment of the proposed Center for Molecular Design and Development (CMDD) at the University of Arkansas at Little Rock (UALR). In particular, as the Director of the UALR Computational Research Center (CRC), I am fully committed to provide computing and data storage service needed by the proposed unit to accomplish research and educational activities associated with the proposed this computational center.

Dr. Darsey's projects require computational resource for performing numerous modeling studies such as procedures to model polymeric and catalytic materials for use in the development of Proton Exchange Membranes (PEM) for fuel cells. Having known his successful career as a computational chemist who can apply computing tools to explore his domain of science, I am confident that Dr. Darsey's team can shed some fundamental insight on a limitation of the diffusion rate of proton $[H^+]$ ions through the polymer membrane, which seems to be considered as a major problem with PEM type fuel cells. He has also had extensive experience with developing new models of catalytic materials. His group has been at the forefront of molecular modeling and there have been many groups which have had collaborations with his group. Another area where Dr. Darsey's group has made significant progress is in the area of drug design. This drug design research has been funded by the Michael J. Fox Foundation for Parkinson's Disease and the U.S. Army Medical Research and Materiel Command.

Our facility currently has a Rocks 5.4 cluster consists of 64 Dell PowerEdge machines (each with 8 Xeon processors and 16GB RAM, for a total of 512 cores), 64TB storage, Gigabit Ethernet, and Infiniband interconnection among computing nodes and a 40TB Lustre parallel file system. It has the theoretical peak performance of 5.45Tflops (or 5.45 trillion floating point operations per second). We also have a big memory server consisting of 80 processors and 4TB of RAM on a single computer as well as a data storage server capable of over 100TB of user data.

Thus, our system environment is equipped with sufficient and ideal computing resource for supporting the mission and operation of the CMDD, and I am fully committed to provide extended access to the student and faculty of the proposed center. Please feel free to contact me if you have any questions.

Sincerely,



Kenji Yoshigoe, PhD
Director of UALR Computational Research Center
Donaghey College of Engineering and Information Technology
University of Arkansas at Little Rock
Phone: (501) 569-8138



May 8, 2014

To Whom It May Concern:

It is my great pleasure to support the efforts of Dr. Jerry A. Darsey, Professor of Chemistry to establish the Center for Molecular Design and Development (CMDD) at the University of Arkansas at Little Rock campus. This center would be a valuable asset for the University of Arkansas at Little Rock as well as other institutions of higher learning in the state of Arkansas.

The exact computational effort of Dr. Darsey's group relates to performing modeling studies on catalytic materials for use in the development of Proton Exchange Membrane (PEM) fuel cells. I am very confident that Dr. Darsey's group can shed some fundamental insight on some of the catalytic materials which can take the place of platinum (Pt) as a material for PEM fuel cells. The major problem with Pt catalyst is that it is very expensive. It will be absolutely necessary to find substitute catalytic materials before a truly commercial fuel cell can be developed. His group has been at the forefront of molecular modeling of such materials. I am also aware of several other groups which have collaborations with Dr. Darsey's group. These collaborations have resulted in numerous presentations at national meetings as well as numerous publications.

Dr. Darsey's group is also engaged in modeling the interactions of bioactive small molecules with the active sites of specific protein receptors. My colleague Dr. Abul B. Kazi is currently working in collaboration with Dr. Darsey's laboratory to explore the p-Glycoprotein binding of paclitaxel analogs using molecular modeling techniques including quantitative structure activity relationship (QSAR) studies. I believe that establishment of the proposed center will greatly enhance their capabilities to perform such studies and will make a positive impact on the quality and outcome of research at the institutions involved.

I, therefore, enthusiastically support the initiative of Dr. Darsey to establish the Center for Molecular Design and Development at UALR.

Sincerely,

A handwritten signature in black ink, appearing to read "Antonie H. Rice".

Antonie H. Rice, Ph.D.
Assistant Dean, School of Arts and Sciences
Chair, Professor
Department of Chemistry and Physics

UNIVERSITY OF
ARKANSAS PINE BLUFF

DEPARTMENT OF CHEMISTRY AND PHYSICS

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June 2, 2014

Dr. Jerry A. Darsey
Department of Chemistry
University of Arkansas at Little Rock (UALR)

Re: Letter of Support

Dear Dr. Darsey,

I am writing this letter to express my support of the proposed new center, "Center for Molecular Design and Development (CMDD)". Having such a Center at UALR would greatly benefit our graduate program in Bioinformatics as well as the Arkansas IDeA Network of Biomedical Research Excellence (<http://brin.uams.edu/>) Bioinformatics core. The proposed Center would give our students and faculty in Bioinformatics better access to simulation, data mining, and visualization techniques for understanding and modeling interactions within complex molecular systems. For our students and faculty in bioinformatics, this translates to better opportunities for solving problems in drug design, computational biology, and personalized medicine. Moreover, bioinformatics researchers across Arkansas will have another key investigational resource in the CMDD that would nicely complement the capabilities of the UALR Emerging Analytics Center, the UALR Computational Research Center, and the UAMS Biomedical Informatics Group for analyzing complex biological data such as genetic codes.

In summary, I heartily endorse the establishment of the Center for Molecular Design and Development at UALR. This Center can count on the full support and participation of the UALR/UAMS Joint Graduate Program in Bioinformatics.

Sincerely,



Elizabeth Pierce
Chair and Associate Professor of Information Science



June 4, 2014

To Whom It May Concern:

I am writing to support the formation of the Center for Molecular Design and Development. This center will have an more impact in building the research capacity of UALR and will also be a nucleus for novel research collaborations both internally and external. Given the current group at UALR as well as nearby UAMS and NCTR, the establishment of this center seems to be an obvious forward-thinking approach to build UALR's research base.

Besides the obvious impacts in research and innovation, this center will have a profound impact on the UALR graduate education productivity. This center will be a resource for high impact graduate student projects and should attract better graduate students and post-doctoral researchers. I envision the center be a part of the Applied Science PHD program mission to provide the foundation for world-class graduate level education.

I am enthusiastic about the Center for Molecular Design and Development and urge the support of Dr. Darsey and this initiative.

Sincerely

A handwritten signature in black ink, appearing to read 'John Bush', is written over the printed name.

Dr. John Bush
Chair of Biology
UALR



OSMANIA UNIVERSITY

*Department of Chemistry
University College of Science
Hyderabad-500007. INDIA.
email: sarathy@osmania.ac.in*

Date: March 28th, 2014.

TO WHOM IT MAY CONCERN

I am writing this letter as one for an extension of support to Dr. Jerry A. Darsey, Professor of Chemistry at the University of Arkansas at Little Rock, and his efforts to develop a Center for Molecular Design and Development. Establishing this center will enhance a better collaboration with respect to both research and academia between Osmania University, Hyderabad, India and University of Arkansas at Little Rock. We can offer significant memory space on our huge servers for the proposed center by Dr. Darsey. This space can be used for joint projects between our two institutions for work related to the structures of polymers and biopolymers. Our research on understanding the kinetics of vinyl polymerization and convergence analysis on the drug candidates need highly efficient QSAR and Docking analysis tools which are available at the proposed center. The efforts made by the group for innovative molecular modeling and computer-based simulation techniques for ligand and structure-based drug design, translational medicine and protein family based approaches to design and identify drug-like compounds, will have far more outreach to the international community. Only with the development of a center with specific aims of computational modeling, will this research be realized. I have great confidence with Dr. Darsey and his expertise in developing computational models for target based drug delivery systems. The center will provide some valuable inputs for both of our laboratories requirements for better models in combating extreme drug resistant and multiple drug resistant tuberculosis which is highly prevalent in India. Furthermore, establishing this center will pave ways for future student exchange programs between Osmania University and University of Arkansas at Little Rock.

I sincerely believe in the need for the proposed center. I and the Department of chemistry, University College of Science at Osmania University support the efforts made to develop a Center for Molecular Design and Development at University of Arkansas at Little Rock.

If you have any questions, please do not hesitate to contact me. My contact information is given below.

Sincerely,


Dr. T. Parthasarathy

Professor of Chemistry,

University College of Science,

Osmania University, Hyderabad – 500007, India.

Phone: +91 40-27682337, +919949652118.

Signature Page

Primary proposer

Date

Department Chair

Date

Dean

Date

Interim Vice Provost and Dean of Graduate School

Date

Provost and Executive Vice Chancellor for Academic Affairs

Date

Chancellor

Date