# EMERSON CENTER Newsletter

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## *Inside This Issue . . .*



### *Letter from Keiji Morokuma*

Effective September 1, I step down as the Director of the Emerson Center as well as William Henry Emerson Professor to become William Henry Emerson Professor Emeritus. I personally have enjoyed and benefited tremendously from the fascinating facilities and atmosphere of the Emerson Center for the last thirteen years. I would like to take this opportunity to thank Emory University, the Emory community, and Emerson Center subscribers and staff members for their support provided to me and to the Center. The Emerson Center was established in 1991 with a generous gift from Dr. Cherry L. Emerson with two goals: 1) to provide high-end computational facilities and expertise in support of research in scientific computation at Emory, and 2) to propel Emory to the world's forefront of computational sciences. On the first goal, the Center has been able to provide state-of-the-art hardware and outstanding expertise in hardware, software and computational techniques. On the second goal, the Emerson Center subscribers published about four hundred papers in the last six years alone based on the work performed using the Center facilities. The Center hosted a major international conference in computational chemistry. With combined efforts of the subscribers, Emerson Center is now a very well known center of computational science in the world. As Emory starts its new Computational and Life Sciences Initiative to establish a community that integrates the traditional science disciplines in exciting new ways, much more opportunities seem to lie ahead for further development of the Emerson Center. I ask for your continued support to the Center.

## Emerson Center's New Structure

*Vaidy Sunderam, Chair, EC Leadership Committee*

The Emerson Center was established in 1991 through a generous gift from Dr. Cherry L. Emerson. Prof. Joel Bowman served as Acting Director and was succeeded by Keiji Morokuma as Director in 1993. Under their leadership, the EC has grown and contributed greatly to computationally oriented science at Emory. Keiji's retirement after 13 years at the helm will surely leave a void, and it will be hard to replace him. A committee structure has been set up to take on the responsibilities previously held by Keiji, and a brief description follows.

The Emerson Center Leadership Committee (ECLC) was appointed by the Dean of Emory College Bobby Paul in Spring 2006 to manage and guide the operation of the Emerson Center. It comprises one faculty representative each from Biology, Chemistry, Math & CS, and Physics, among whom chairmanship will rotate every 3 years. The previous position of EC Manager has been retitled Director for titular alignment with other centers; the director serves ex-officio on the ECLC.

Professors Dieter Jaeger (Biology), Joel Bowman (Chemistry), Vaidy Sunderam (Math & CS), Kurt Warncke (Physics) and Jamal Musaev (ex-officio) are the 2006-2009 ECLC members, with Vaidy Sunderam serving as Chair. This committee pledges to continue building upon the excellent work of the previous directors, and to serve EC subscribers to the best of their ability. We hope to work closely with subscribers and with researchers as well as University units to facilitate the best possible computational research and scholarship. The ECLC, ably assisted by Jianli Zhao and Alex Kaledin, aims to be highly responsive to subscriber needs and will be proactive in growing the subscriber base, enhancing the visiting fellows and symposium programs, proposing new initiatives and acquiring enhanced equipment and software. We look forward to a close and productive relationship with subscribers and the computational community at large.

## EC Welcomes New Subscribers

*Emerson Center welcomes Dr. Dale Edmondson, Professor of Biochemistry and Chemistry, as the newest subscriber to the Emerson Center. The research focus of Dr. Edmondson's laboratory involves investigations of structure-function relationships in enzymes catalyzing oxidation-reduction reactions. Among the enzymes belonging to this class, particular emphasis is given to the flavoenzymes, monoamine oxidases A and B, (MAO A) and (MAO B), respectively. Several of these enzymes are important targets in the development of drug therapies such as antidepressants (monoamine oxidase). The MAO A and MAO B project involves structure-activity studies to probe the structure of the amine binding site and to probe the detailed mechanism of oxidative deamination of amine neurotransmitters. Ongoing work includes the determination of the structure of MAO A and the investigation of site directed mutants of both MAO A and MAO B to probe their mechanisms of amine oxidation and the binding of antidepressants and neuroprotective agents to the catalytic centers of each enzyme. Dr. Edmondson plans to use the Emerson Center facilities to expand his computational studies (starting with a collaboration with Drs. Rajeev Prabhakar, Jamal Musaev and Keiji Morokuma) on the mechanism of amine oxidation and the binding of antidepressants and neuroprotective agents to the catalytic centers of each enzyme.*

*Prof. Dale Edmondson*

## Letters from Fellows

*During my stay as an Emerson Center visiting fellow at Emory University I had a very wonderful and enjoyable time thanks in part to the kindness of Professor Morokuma and Dr. Musaev and, in particular, to Ms. Jianli Zhao who was extremely helpful in solving my housing and all the paperwork problems a foreign visitor like me have to overcome. I have to say, though, that I was not a newcomer to the EC for I was a post-doc in Professor Morokuma's group from 2002 to 2004. It was very nice to work again with Professor Morokuma and Dr. Musaev and, as a result, to have very fruitful discussions regarding my single-walled carbon nanotube project. My research at the EC was mainly focused on doped SWCNT, which is a promising approach for controlling the electronic structure and it is technologically very important for the practical device manufacturing in order to increase lithium ion battery performance.*

*Dr. David Quinonero*

*After this brief report I would like to share with you how amaze I was when I saw the change Atlanta has experienced in the last two years, a city in continuous construction (Midtown is an example) and rejuvenation, like the Little Five Points area.*

*Finally, I would like to thank all the people who made my pleasant stay possible and, especially, the great initiative to do research which represents the Emerson Center Visiting Fellowship program for giving me the chance to visit this great center.*

*David Quinonero*
*Department of Chemistry*
*Universitat de les Illes Balears Spain*

*Dr. David Quinonero visited Emory as an Emerson Center Visiting Fellow in October 2006.*

## EMERSON CENTER VISITING FELLOWSHIP

*The Emerson Center offers visiting fellowships to interested scientists throughout the year. Scientists from academic institutions all over the world who want to perform intensive research in computational chemistry, biology, physics, and math & computer sciences for one to several months are encouraged to apply. Travel expenses and stipends are available. Although fully independent research is not excluded, collaboration with an EC subscriber is desirable, and EC subscribers are encouraged to make recommendations. The deadline for Emerson Center Visiting Fellowship applications for summer 2007-summer 2008 is February 1, 2007. To formally apply, please submit:*

- *1-2 page research proposal*
- *CV including publication list*
- *Amount of financial support needed*
- *Length of stay with an approximate start/end date*

*Applications should be submitted to the Emerson Center (address on p. 4).*

***APPLICATION DEADLINE: February 1, 2007***

## My Stay at the Emerson Center as a Visiting Fellow

*Hao Wang, Ph.D., Dept. of Physics, Nankai University, China*

As a physicist, my interest gradually switched from pure physics to biophysics recently, because I found that in bio-systems there are tons of natural physical problems awaiting to be solved. So I decided that I should find a position and do something very different from what I had been doing.

So in mid-August of 2005, I drove 1,300 miles from Fargo, North Dakota to the hot and humid city of Atlanta, to take a position sponsered by the Emerson Center Visiting Fellowship program at Emory University. My host was Prof. James T Kindt, one of Emerson Center's subscribers.

*Dr. Hao Wang*

A major rearch interest of James' group is simulating lipid membranes, where cusomrized MCMD(Monte Carlo+Molycular Dynamics) simulations have been carried out on those big computer clusters run by Emerson Center. Simulating systems consisting of lots of particles that involve complex interactions is always a challenge. People rely on simple theoretical models for predicting the properties of systems that is beyond the present computing capabilities. That's what James and I have been trying to do — study phases coexistence of various structures in lipids mixtures. We have seen some very interesting results and are looking forward to more.

To summarize, I want to say thanks to Dr. Morokuma, Dr. Musaev and Dr. Irle for their hospitality, and to Jianli Zhao who helped me go through administrative things easily so that I could focus on my research.

*Dr. Hao Wang stayed at the Emerson Center as a Visiting Fellow from August 2005 to April 2006.*

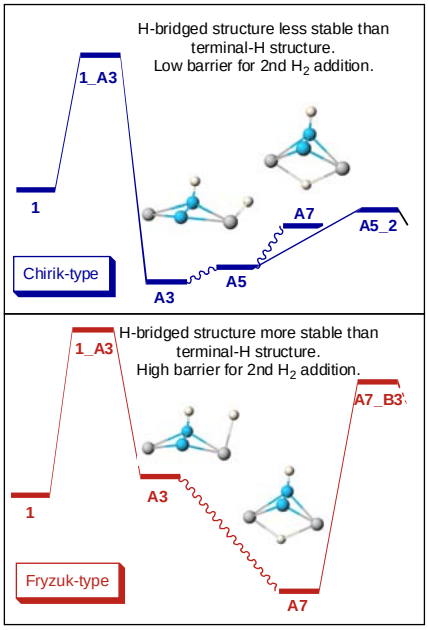
# *Report on Research Activities at the Emerson Center*

*The Emerson Center is supported, in part, by "subscribers" - faculty members, research groups or departments that purchase shares in order to gain access to its resources for their research projects. EC scientific staff members are also encouraged to conduct scientific research in their own areas of specialty. The following are two research reports from the Emerson Center.*

## Seeking New Catalysts For Hydrogenation Of Nitrogen Molecule At Mild Conditions

*Petia Bobadova-Parvanova, Keiji Morokuma, & Djamaladdin G. Musaev*
*Cherry L. Emerson Center and Department of Chemistry*

*Industrial hydrogenation of the nitrogen molecule is an extremely important and widely used catalytic process, necessary for the production of fertilizers, fuels, and dyes. It produces more than 100 million tons of ammonia annually and is responsible for sustaining around 40% of the word's population. The currently used catalysts require extreme temperature and pressure. Although a new catalyst that could transform $N_2$ under mild conditions has been sought for more than 70 years, a breakthrough discovery has not yet been made. Such a discovery would have a great impact on the U.S. and world economy.*




*Potential energy profile of addition of two H2 molecules to Chirik- and ryzuk-type of complexes*

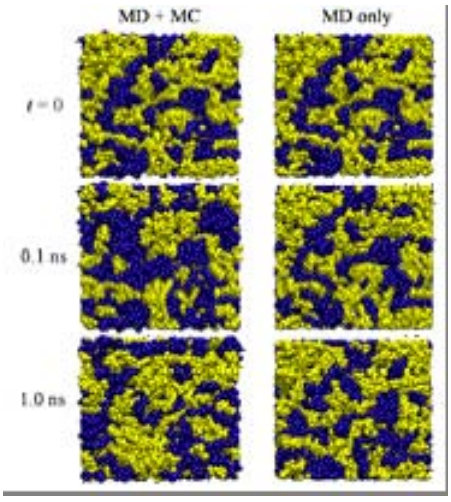
*For the last several years the Morokuma and Musaev group has been a leader in the field of theoretical modeling of promising reactions for successful $N_2$ hydrogenation under mild conditions. In a recent publication (*JACS ***2006***, 128, 11391), postdoctoral researcher Petia Bobadova-Parvanova applied first-principle calculations to study the mechanisms of $N_2$ hydrogenation by two different complexes – one synthesized by Chirik and co-workers [*Nature ***2004***, 427, 527] and another synthesized by Fryzuk and co-workers [*Science ***1997***, 275, 1445]. The former complex is experimentally known to be capable of adding more than one $H_2$ molecule and eventually producing ammonia, while the latter does not add more than one $H_2$. Theoretical modeling has shown that the experimentally observed difference in the reactivity of these complexes is caused by the fact that the former ligand environment is more rigid than the latter. As a result, the addition of the first $H_2$ molecule leads to two different products: a non-H-bridged intermediate for the Chirik-type complex and a H-bridged intermediate for the Fryzuk-type complex (see figure). The non-H-bridged intermediate requires a smaller energy barrier for the second $H_2$ addition than the H-bridged intermediate. The authors have also performed an extensive analysis on the factors (side-on coordination of $N_2$ to two Zr centers, availability of the frontier orbitals with appropriate symmetry, and the inflexibility of the catalyst ligand environment) that are required for successful hydrogenation of the coordinated nitrogen molecule and thus have given a guide for the synthesis of new complexes with the desired properties.*

## A new approach allows simulation of equilibrium structure in mixed lipid bilayers

*James Kindt, Department of Chemistry*
*Emory University*

A typical cell membrane contains a complex mixture of lipid molecules whose specific composition is carefully regulated by the cell. To understand what roles the many lipid components are playing, we need to learn how they are arranged – how their molecular structures influence whether are spread uniformly through the membrane, form domains or "rafts" with similar lipids and cholesterol, or cluster around particular proteins.

Molecular simulation would seem to be an ideal tool to study this behavior, except that the exchange of lipids among different environments is too slow to observe during a typical simulation that can model 10's of nanoseconds of lipid dynamics. Using a version of the Gromacs simulation package customized by postdoc Jason de Joannis, we have shown that a mixed molecular dynamics-Monte Carlo (MD + MC) approach using controlled mutations of lipids from one type to another can overcome this limitation. We have seen a roughly 100-fold increase in efficiency of mixing over pure MD, as evident from simulation snapshots of a mixed-lipid bilayer shown in the figure, where DPPC lipids are colored blue and DLPC is colored yellow. The method has been applied to measuring the equilibrium occupation ratios of two different lipid types at a bilayer edge defect and at specific sites surrounding a trans-membrane helical peptide. Further work will expand the range of lipid mixtures that can be treated, and will investigate ternary mixtures including cholesterol. The simulations have been carried out largely on the Emerson Center's Sun Linux Opteron cluster. Many members of the Kindt group have contributed to running and analyzing the simulations: graduate students Frank Yong Jiang and Fuchang Yin, postdoc Hao Wang, and Emory College students Jeff Gaulding ('06), Kunal Khanna ('07), and Kanwei Li ('08).




*Snapshots from simulation of mixed-lipid bilayer containing DPPC (blue) and DLPC (yellow), comparing evolution of distribution with and without Monte Carlo mutation moves*

## The EC Lectureship Award Symposium Series Continues to be Successful

The 3rd Emerson Center (EC) Lectureship Award Symposium on the "Computational and Mathematical Modeling in Large Systems: From Proteins to Cells" concluded successfully on April 3, 2006. In spite of the heavy rain, more than 130 people, including faculty, students and postdocts from Emory, Georgia Tech (27 people), University of Georgia (9), Georgia State University (7), University of Alabama at Birmingham (6), University of Tennessee at Vanderbilt (7), University of Clemson (4), Spellman College (2), Coca-Cola Company (2) and Kennesaw State University (1) attended this one-day event.

Dr. Earl Lewis, Provost of Emory University, opened the event by emphasizing the importance of this Symposium series for the Emory Community in bringing together prominent scholars with different scientific backgrounds and helping the promotion of cutting-edge research activities at the university. Prof. Lanny Liebeskind, Director of University Science Strategies, expressed his gratitude to the EC Lectureship Award Selection Committee and Emerson Center staff for their marvelous job in organizing this event.

This year's keynote speaker was Prof. Martin Karplus of Harvard University (USA) and ISIS Universite Louis Pateur (France). Prof. M. Karplus highlighted recent advances in computational and mathematical modeling of protein action. He pointed out that living cells are a collection of molecular machines, which carry out many of the functions essential for the cells' existence, differentiation and reproduction. Most, though not all, of these machines are made up of proteins. Because of their complexity, an understanding of how they work requires a synergistic combination of experimental and theoretical studies. The specific focuses of Prof. Karplus's presentation were molecular motors GroEL and F1-ATPase.

Five other renowned scholars including Professors Dieter Jaeger (Emory, Biology), Steve Harvey (Georgia Tech, Biology), David Lynn (Emory, Chemistry & Biology), Kurt Warncke (Emory, Physics)), and Ying Xu (UGA, Biochemistry and Molecular Biology) presented the latest developments in their laboratories.

The poster session, featuring latest research findings of students and postdocts from varies universities and colleges of the southestern states, was lively with intensive scientific discussions. Two "Best Poster Award" awards ($100 each) was awarded to Dr. Andrea Catte of University of Alabama at Birmingham, and Dr. Thomas Caulfield of Georgia Tech.

Dr. Jamal Musaev, Manager of the Emerson Center and Lectureship Coordinator, and Prof. Kurt Warncke, Chair of the EC Lectureship Committee, expressed their appreciation to all Participants, Subscribers, Lectureship Committee members, EC staff, and Speakers. Dr. Cherry L. Emerson, EC's benefactor, attended to all presentations and the special dinner honoring Prof. Martin Karplus.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***This issue of the Emerson Center Newsletter is designed and edited by Jianli Zhao***


## EC Hardware/Software Report

*Drs. Jamal Musaev & Alex Kaledin, Emerson Center*

### * Installation of new software on IBM SP and Sun Fire

*As part of our steady upgrade of the Center's computational resources, we have added the following software on both the IBM SP and Sun Linux clusters. GAMESS 06 (parallel) interfaced with TINKER 4.2 for flexible description of solvent effects on molecular interactions; MOLPRO 2006.1 featuring a new implementation of QCISD(T) gradient, the symmetry-adapted intermolecular perturbation theory for studying cluster interactions, and linearly scaling 'local' MP2 and CCSD theories; DALTON 2.0, suitable for high accuracy spectroscopic predictions; ACESII(M) version from the developers in Mainz, Germany, featuring an efficient CCSDT analytic gradient; MATLAB 2006a version 7.2.0 & Mathematica 5.2; Finally, the newly released PGI 6.1 FORTRAN compiler has been installed on the Linux cluster.*

*EC 2006 Lectureship Symposium Speakers, left to right, M. Karplus, S. Harvey, D. Jaeger, D. Lynn, K. Warncke, and Y. Xu*