EMERSON CENTER Newsletter

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http://www.emerson.emory.edu
Volume 13, March 15, 2004

Inside This Issue . . .

◆ *Dept. Subscriptions at Work for Research, Courses & Fellowships*

The Emerson Center is supported in part by subscription fees paid by subscribers. There are two categories of subscriptions. One is an individual subscription for Emory faculty who uses the Center's facilities for his/her own research. The other one is a departmental subscription; presently Chemistry, Math & Computer Science, and Physics Departments are departmental subscribers. Members of subscribing departments are entitled to receive full services from the Emerson Center, like individual subscribers. Different departments are interested in somewhat different services. While one department may be interested primarily in the Visiting Fellows program, another department takes advantage of the center's resources (hardware, software, and consulting) to meet the computational needs of its faculty members. Chemistry Department, for example, uses the EC facilities for research activities of its non-tenure faculty members and for courses such as Chem430, Undergraduate Computational Chemistry, and several of graduate level courses. In those courses, the SP2 computer system at the Center becomes very handy; although its speed is considerably slower than SP3 and SP4 systems, this particular queue is available all the time without wait, making it a great teaching resource. Moreover, students have full access to the Center's rich software library and compilers.

EMERSON CENTER LECTURESHIP SYMPOSIUM

The first annual Emerson Center Lectureship Award Symposium will be held on May 1, 2004, in Atwood Hall (Chemistry Building) of Emory University. Announcements for the symposium were sent to about 100 colleges and universities in Georgia and surrounding states. The Award Winner/Keynote Speaker for this year's symposium is Dr. William A. Goddard, III, internationally recognized professor of chemistry and applied physics of California Institute of Technology. His talk will highlight some recent advances in methodology and will illustrate them with recent applications to problems involving Proteins, DNA, Polymers, Ceramics, Metals, Semiconductors, and Catalysis. Please refer to the inserted flyer for symposium details.

Prof. William A. Goddard, III

The Emerson Center Lectureship Award was established in fall 2003 to promote the Emerson Center Subscribers' scientific interests, bring more domestic and international recognition to the center and Emory University, recognize distinguished achievements by scientists in computational sciences and to facilitate collaboration among different disciplines of computational sciences. The Selection Committee, which includes representatives of five Departments (Biology, Biochemistry, Chemistry, Mathematics & Computer Science, and Physics) as well as the Emerson Center, will select once a year a scientific field and one of the leading scholars of this field for lecture presentation at the Emerson Center, based on nominations by EC Subscribers. An annual one-day symposium with participation of students, postdocs and faculty from neighboring colleges/universities will be held; speakers of the symposium will be the lectureship winner and local scholars.

The members of the Selection Committee for 2003-2006 are: Profs. Rustom Antia (Biology), Michele Benzi (Math & Comp. Sci.), Justin Gallivan (Chemistry), Keiji Morokuma (Emerson Center), Kurt Warncke (Physics), and Keith Wilkinson (Biochemistry). Dr. Jamal Musaev, Manager of the Emerson Center, is the Coordinator for the Lectureship.

NEW EXECUTIVE COMMITTEE APPOINTED

A new Emerson Center Executive Committee was appointed in the early Spring of 2004 by Emory College to serve a 3-year term. The center's Executive Committee was originally established in 1998 based on recommendation of the five-year review committee of the Emerson Center in the Fall of 1997 as an overseeing committee of the Center's operations. The new committee members are professors representing the various disciplines of the Emerson Center subscribers. They are Profs. Rustom Antia (Biology), George Hentschel (Physics), David Lynn (Chemistry), Keiji Morokuma (Emerson Center, Chair), Vaidy Sunderam (Math & CS), and Keith Wilkinson (Biochemistry). Prof. Joel Bowman, current Chair of the Chemistry Department, serves as ex officio.

Letters from Fellows

Last summer I spent 3 exciting months as a Visiting Fellow at the Emerson Center. My research interest in studies of mechanisms of enzymatic reactions using isotope effects led me to QM/MM techniques, and this visit allowed me to learn in-home tricks of the ONIOM approach that was introduced by my host, Professor Keiji Morokuma. Simultaneous stay of my student in the same lab allowed us to apply this method to two different enzymatic systems: a dehalogenase and a mutase. While both of these projects proved much more time consuming than we originally anticipated there is no question that they could never be started if we hadn't have the occasion to discuss all the problems with Prof. Morokuma and a number of his associates. Great computational facilities allowed us to move on with these projects and I hope this collaboration, which is already so fruitful, will continue in the future. But the experience gained at the Emerson Center is not only restricted to these particular two projects. I have found seminars and meetings most educational and the whole atmosphere of the place very inspiring and research promoting. As a volleyball addict I have also found a group of people who introduced me to wallyball. Both these scientific and recreational aspects summed up to fantastic yet extremely productive time that I had in Atlanta. I wish every summer was like this one!

Dr. Piotr Paneth at EC

Prof. Piotr Paneth Ph.D., D.Sc.
Technical University
Lodz, Poland

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Dr. Piotr Paneth visited Emory as an Emerson Center Visiting Fellow from June to October 2003.

Emerson Center Visiting Fellowship Awards for 2004-2005

Ms. Biggi Albrecht, *University of Oxford, UK*
Dr. Jacques G. Amar, *University of Toledo, USA*
Dr. Valentin P. Ananikov, *Russian Academy of Sciences, RUSSIA*
Dr. Carl T. Bergstrom, *University of Washington, USA*
Dr. Wafaa M. Fawzy, *Alexandria University, EGYPT*
Dr. Maciej Malawski, *Institute. of Comp. Sciences, POLAND*
Dr. Minh Tho Nguyen, *University of Leuven, BELGIUM*
Dr. Josep M. Poblet, *University of Rovira i Virgili, SPAIN*
Dr. Edward Rosenberg, *University of Montana, USA*
Dr. Suwipa Saen-oon, *Chulalongkorn University, THAILAND*
Dr. Tetsuya Taketsugu, *Ochanomizu University, JAPAN*
Dr. Trina Valencich, *University of Montana, USA*
Dr. Shucheng Xu, *Emory University, USA*

The Emerson Center offers visiting fellowships to interested scientists throughout the year. Please refer to the Emerson Center homepage at http://www.emerson.emory.edu for application details and deadlines, or send email to clec@euch4e.chem.emory.edu.

My Stay at the Emerson Center as a Visiting Fellow

Dr. Seung C. Park, Professor of Chemistry, Sungkyunkwan University, Suwon, Korea

It is a great pleasure and privilege for me to be visiting Emerson Center at Emory for my sabbatical leave. The advantages of a sabbatical are not only the privilege to work in a new environment, which stimulates scientific research, but also the opportunity to experience a different culture. This is a unique experience in my life and for my family.

I have the opportunity of collaborating with Prof. Joel Bowman, gathering new scientific knowledge and opening my research to new fields and interests. We are working on the reaction dynamics of the bimolecular polyatomic reaction, particularly, $O(^3P) + C_3H_3 \rightarrow OH + C_3H_2$ reaction. This reaction is important not only as a fundamental reaction to organic chemistry, but also in atmospheric and combustion chemistry. The goal of the work is to understand the OH formation dynamics in the reaction. For this purpose, we are developing a new method for constructing a potential energy surface for general polyatomic reactions that is a challenging work to the multi-dimensional system. The general code for the bimolecular reaction dynamics is also developed which enables us to perform the $O(^3P) + C_3H_3 \rightarrow OH + C_3H_2$ reaction.

The Park Family in Atlanta

Beside science, my family and myself are enjoying a different environment and a different culture. The city of Atlanta has unique features, compared to other big cities that I have experienced. The city has lots of greens and woods that are very rare in usual big cities. My family enjoys the green space and the woods and the peacefulness they bring to us. The cultural activities in the city are very vital. Atlanta has a world-class orchestra and a high level of Opera Theater. My family enjoys high quality performing arts that are the benefits in living in Atlanta.

My deep gratitude goes to Professor Bowman and to the members of the Bowman group for the many stimulating discussions as well as for the help that I received during my stay at Emory. I am very grateful to acknowledge Professor Keiji Morokuma and Cherry L. Emerson Center for allowing me the visiting fellowship. I look forward to future occasions for visiting such a wonderful place.

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Dr. Park has been a visitor of the Emerson Center since Aug. 2003 and will return to Korea at the end of his sabbatical in late July 2004.

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 research reports from two subscribing groups at the Emerson Center.

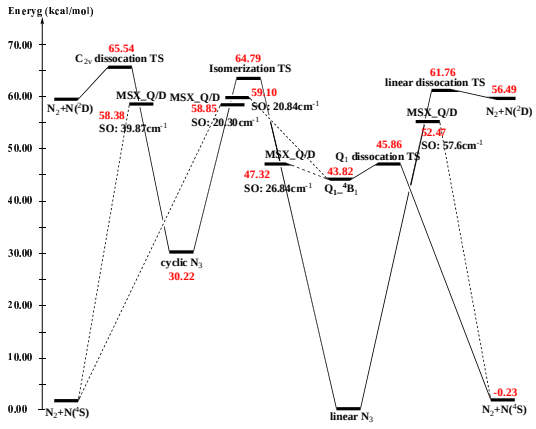
Theoretical Investigation of the Ground State N_3 Radical

Peng Zhang and Keiji Morokuma
Chemistry Department and Emerson Center

Because of their large exothermicity in decomposition reaction, nitrogen clusters have been vigorously sought as materials capable of storing large amounts of energy in minimal volumes, the so-called "high energy and density materials". Their natural tendency to decompose to N_2 also makes them high on the list of environmentally friendly propellants and explosives.

During the last decades, tremendous efforts have been made in synthesizing and understanding this new class of molecules. The early study in the Morokuma group regarding the stability of this type of nitrogen clusters can be traced back to 1995, when the Woodward–Hoffmann forbidden dissociation of tetrahedral N_4 to $2N_2$ was explored with molecular orbital calculations. Recently, high-level calculations predicted the existence of cyclic-N_3 that may undergo barrierless exothermic recombination with $N(^2D)$ to form tetrahedral N_4. This makes cyclic-N_3 one of few suggested precursors to tetrahedral N_4. Therefore, theoretically understanding the relative stability and the corresponding dissociation dynamics is essential in guiding practical applications.

In recent calculations, Peng Zhang, a fourth year graduate student, and Keiji Morokuma have characterized potential energy surfaces of N_3 radical both in linear and cyclic regions using the very accurate multireference configuration interaction method. These high-level theoretical calculations, carried out on the IBM-SP4 computer at the Emerson Center, were a critical component in understanding this chemistry. The calculated potential energy profile of N_3 radical is shown in the figure. Linear N_3 is the global minimum on the lowest doublet state, and another isomer, cyclic-N_3, lies 30.2 kcal/mol above it and the isomerization barrier from linear to cyclic form is about 64.8 kcal/mol. Calculations suggest that the formation of linear isomer from $N(^2D)$ with N_2 could be easier than that of cyclic isomer. In addition, five minima of seam-of-crossing (MSX), contributing to the non-adiabatic from the doublet to a quartet state that leads to dissociation, have been located at different regions of potential energy surface. These results suggest that the fragmentation dynamics of the cyclic isomer is nonadiabatic. Beside the ground state investigation, a series of calculations have been carried out on the electronically excited states, which could provide the information for photodissociation dynamics and for designing the experiment of detecting and synthesizing the cyclic-N_3. The present work was carried out in collaboration with Prof. Alec Wodtke of University of California, Santa Barbara, who performed experimental studies, and was supported by a grant from the US Air Force Office of Scientific Research.



Computing the Free Energy of Vesicle Formation

Research report by Dr. James Kindt
Assistant Professor, Chemistry Department

Although molecular dynamics simulation is a powerful tool, many interesting phenomena encompass system sizes and time-scales that lie beyond the reach of molecular simulation methods, and require a coarse-grained or mesoscale treatment. Dr. Shi-Jin Zhao in the Kindt group is using a mesoscale model, to investigate how large a membrane fragment will grow before closing on itself to form a closed shell, or vesicle. This transition is governed by two energies: the energy penalty of the membrane edge, which is proportional to the perimeter of the membrane fragment, and the bending energy, which is roughly independent of vesicle size. In addition to producing fascinating structures (like the vesicle depicted in the figure) Dr. Zhao's Monte Carlo simulations yield a free energy landscape for the process of membrane growth and vesicle formation. Recent results suggest that the perimeter of the membrane fragment is proportional to the area raised to the four-fifths power - not the square root of the area as one would predict for a perfectly flat, round disk. The next stage in this study will be to use the results and scaling relations to predict and rationalize experimentally observed vesicle size distributions.

Recent EC Software Upgrades

Drs. Jamal Musaev & Stephan Irle, Emerson Center

The EC has recently upgraded a number of its software packages, which we would like to describe here in more detail. For questions on these and other software packages available at the Center please visit our website at http://www.emerson.emory.edu/Cover/software.html.

Gaussian 03 Revision B.5: Upgrade from previous G03BX and AX versions. LoadLeveler (LL) submission scripts are only available for SP3 and SP4 systems and can be found in /libs/scripts/g03/g03b5sp3 and /libs/scripts/g03/g03b5p4. While new features of G03 can be found at Gaussian's website at http://www.gaussian.com, we would like to emphasize the possibility of using Gaussian as master program e.g. in ONIOM type calculations with other programs dealing with individual ONIOM levels through the Gaussian keyword "external". Scripts have been written which allow the Emerson Center Gaussian suite of programs to connect to other quantum chemical software packages installed at the EC, such as MOPAC, CADPAC, MOLPRO, and TURBOMOLE both interactively and in LL batch jobs. For instance, for an ONIOM calculation using MRSDCI:MP2:HF one would replace MRSDCI with "external", where a script called "Gau_External" would start MOLPRO calculations of the high level model calculations. This not widely publicized keyword gives the user greater flexibility in ONIOM calculations and allows to take advantage of Gaussian's efficient geometry optimizer for programs which do not possess geometry optimizers of their own.

NWChem 4.5: Newly installed. Allows sequential and parallel (4 processor) jobs using the LL submission scripts /libs/scripts/nwchemrun and /libs/scripts/nwchemprun. NWChem is a computational chemistry package that focuses on highly efficient use of parallel supercomputers, and the installation at the EC can provide important input testing and smaller problem application runs. It has a nice graphics visualization tool called ECCE which is also installed at the EC. NWChem has been developed by the Molecular Sciences Software group of the Theory, Modeling & Simulation program of the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL).

Mathematica 5.0: Upgrade from version 4.0. The EC has purchased copies for 64-bit UNIX (AIX, IRIX), 32-bit LINUX, and MacOSX 10.2 or higher. The LL submission script for batch job Mathematica runs is now called /libs/scripts/math50run. Only SP3 and SP4 architectures are supported. Enhancements throughout make Mathematica 5 better suited to production-scale work than ever

Software, continued on the right--

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This issue of the Emerson Center Newsletter is designed and edited by Jianli Zhao

Hosting a Short-Term Visitor?

The Emerson Center may be able to help you house your short-term visitor. We have a long-term lease on a 2-bedroom/2-bathroom apartment at the Clairmont Campus for the Center's visiting fellows. The apartment has vacancies from time to time and we would be happy to make the space available to other short-term visiting faculty on campus. The apartment has easy shuttle access to campus and is fully furnished with cable TV and internet access. The current rent, which includes all utilities and local telephone service, is $690 per room per month, or $35 per day if less than 30 days. Please call 727-0867 or email jzhao@emory.edu for more information.

--Software, continued

before. It offers a complete solution from initial calculations through prototyping to final solutions and documentation. Information on new features concerning performance enhancements, numeric and symbolic computations, and other functions, can be found at Mathematica's website at http://www.wolfram.com/products/mathematica/newin5/.

AMICA: Newly installed. Based on COLUMBUS, AMICA allows EC subscribers to carry out the supposedly most accurate quantum chemical molecular electronic structure calculations after Full CI calculations using r12-explicitly correlated wavefunctions. It has only been compiled for the SP4 and its LL script is called /libs/scripts/amicarunsp4. Information on this program package can be found at its homepage http://gdanitz.hec.utah.edu.

News from the ECEC Meeting

The 17th meeting of the Emerson Center Executive Committee (ECEC) was held on Monday, Feb. 23, 2004. On the agenda were administrative and technical reports, the Emerson Center Lectureship Symposium, and the 2004-2005 Visiting Fellowship awards. Prof. Keiji Morokuma, Chair of the ECEC, introduced new committee members as they begin their three-year term on the committee and the scientific staff of the center reported on software upgrades and hardware updates at the center. Dr. Jamal Musaev, Manager of Emerson Center and Coordinator of the EC Lectureship Award Symposium, reported on progress of the symposium, its location and the Center's publicity efforts. Dr. Morokuma presented the committee with the list and application files for the 2004-2005 Visiting Fellowship awards, pointing out especially those that have gained support from the center's subscribers. The committee examined each application carefully and made awards to thirteen applicants out of the twenty-five applications received. The research areas of the award recipients range from biology to chemistry, physics, and computer sciences. See page 2 of this newsletter for a list of the award recipients and their affiliations.

EMERSON CENTER LECTURESHIP AWARD SYMPOSIUM

Interface of Computers with Chemistry, Physics, Biology & Materials: Methods & Applications

Cherry L. Emerson Center for Scientific Computation, Emory University

Dr. Cherry L. Emerson

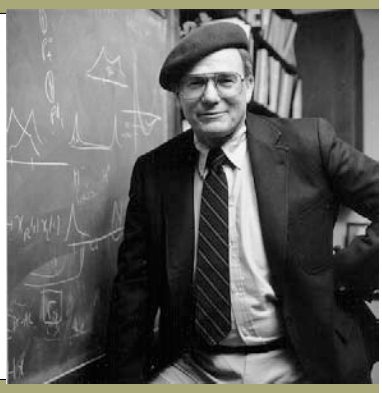
Saturday, May 1, 2004

Location: 360 Atwood Hall, Emory University

AWARD WINNER & KEYNOTE SPEAKER:

William A. Goddard, III

Charles and Mary Ferkel Professor of Chemistry, Materials Science, and Applied Physics
Director, Materials and Process Simulation Center (MSC), California Institute of Technology



We will highlight some recent advances in methodology and will illustrate them with recent applications to problems involving Proteins, DNA, Polymers, Ceramics, Metals, Semiconductors, and Catalysis. This lecture will have three parts: (1) strategy and tactics in applications of the methods to a range of practical problems involving materials science, catalysis, and nanotechnology: (2) recent advances in protein folding and drug design with applications to structure and function of Protein Coupled Receptors (GPCRs), including the receptors for smell, taste, dopamine, epinepherin, histamine, and pain, and (3) details of methods used in the applications presented in Parts 1 and 2.

INVITED SPEAKERS:

Stefan Boettcher
Dept. of Physics, Emory University, Atlanta

Rigoberto Hernandez
School of Chemistry & Biochemistry, Georgia Tech., Atlanta

James Kindt
Dept. of Chemistry, Emory University, Atlanta

Jamal Musaev
Emerson Center, Emory University, Atlanta

Steven J. Stuart
Dept. of Chemistry, Clemson University, Clemson

SCHEDULE OF EVENTS:

9:30 - 9:50	WELCOME & AWARD PRESENTATION
9:50 - 11:00	Prof. William Goddard (CalTech, California), ***De Novo Multi-Scale Simulations Applied to Materials (Polymers, Ceramics, Metals, Semiconductors), Catalysis, Proteins, and DNA***
11:00 – 11:50	Prof. James Kindt (Emory Univ., Georgia), ***Molecular and Mesoscale Modeling of Membranes***
11:50 – 1:30	LUNCH (and tour of Emory and Emerson Center)
1:30 – 2:20	Prof. R. Hernandez (Georgia Tech., Georgia), ***The Role of the environment in Dense Polymerization, Protein Motion and Binding***
2:20 – 3:10	Dr. Jamal Musaev (Emory Univ., Georgia), ***Computational Designing of Catalytic Processes: From the Transition Metal Cations and Clusters through Organometalic Complexes to Enzymes***
3:10 – 3:30	COFFEE BREAK
3:30 – 4:20	Prof. Steve Stuart (Clemson Univ., S. Carolina), ***Bond-Order Approaches for Reactive Materials Science Simulations***
4:20 – 5:10	Prof. Stefan Boettcher (Emory Univ., Georgia), ***Low-Energy Excitations in Very Large Hyper-cubic Spin Glasses in d=3 to d=7***
5:10	Closing
6:00 – 8:30	DINNER (by invitation only)

REGISTRATION AND CONTACT INFORMATION:

Email: clec@euch4e.chem.emory.edu
http://www.emerson.emory.edu/local/register.html
1515 Dickey Drive, Atlanta, GA 30322
Phone: 404-727-2380; Fax: 404-727-7412
Registration is free, but you must register to attend.

The Emerson Center Lectureship Award was established in fall 2003 to recognize distinguished achievements by scientists in computational sciences and to facilitate collaboration among different disciplines of computational sciences. On the board of the Emerson Center Lectureship Award Selection Committee are Professors Kurt Warncke (Physics, chair), Rustom Antia (Biology), Michele Benzi (Math & Computer Science), Justin Gallivan (Chemistry), Keiji Morokuma (Emerson Center), and Keith Wilkinson (Biochemistry) of Emory University. Dr. Jamal Musaev (Emerson Center) is appointed as the Lectureship Coordinator.

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