

# EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation  
<http://www.emerson.emory.edu>  
Volume 6, Sept. 10, 2000

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## In the News

◆ Professor William Miller, Kenneth S. Pitzer Distinguished Professor, UC-Berkeley, spent four months as a distinguished Emerson Fellow. He gave several very stimulating lectures on quantum and semiclassical theories of chemical reactions. His office door was open to all, except when he was out playing squash. He and his wife, Margaret Ann, explored the areas in and around Atlanta, uncovering their family histories. See page 2 for a letter from Prof. Miller.

◆ The Emerson Center webpage will receive a facelift soon. A new design is underway, and viewers will be able to surf the new pages with enhanced capabilities in early fall.

◆ The Emerson Center has received more than a dozen formal applications for the 3rd staff position specializing in modeling and graphics. Review of the applications is underway, and an appointment is scheduled for Fall 2000.

◆ The faculty search for an assistant professor in theoretical/computational chemistry has been re-opened for Fall 2000. Review of applications will start in October.

## Emerson Center Receives NSF Funding for Major Equipment Purchase

Emory University recently received a Major Research Instrument (MRI) grant of \$300,000 from the National Science Foundation for the purchase of new computer systems for computational chemistry and chemical physics at the Emerson Center. The Principal Investigator of the grant is Dr. Keiji Morokuma, Director of the Center, with a team of co-investigators consisting of Emerson Center subscribers and their collaborators (Drs. Joel Bowman, Michael Heaven, M. C. Lin, Dennis Liotta and James Snyder from the Chemistry Department and Drs. Fereydoon Family and George Hentschel from the Physics Department) and Emerson Center scientific staff (Drs. Stephan Irle and Djamaladdin Musaev), joined by computer scientists (Drs. James Nagy and Vaidy Sunderam from Math/Computer Science Department). With this fund and matching money from Dr. Cherry Emerson's original instrumentation fund, new systems consisting of a mix of clustered workstations and personal computers will be purchased to replace the aging SP2 system of the Center. The new purchase is expected to increase the computing power of the Center's system several times over the present power, and to satisfy the ever-increasing needs of subscribers in the coming 3-4 years. An enhancement in the graphic capability is also scheduled. The new systems, being selected by the Emerson Center Executive Committee, are expected to be installed in the new Cherry Logan Emerson Hall starting in early 2001.



## EC SUBSCRIBER/USERS MEETING PLANNED

The Emerson Center is organizing a meeting of all subscribers, users, NSF co-investigators and potential subscribers to discuss issues related to the major equipment upgrade as a result of the NSF grant. The meeting will also nominate additional members to the Technical Sub-committee which will examine technical data and recommend to the Executive Committee on the acquisition of the new computer systems for the Center. The meeting is scheduled for Thursday, Sept. 14, 2:30-4:00pm, in Room 316 of the Chemistry Building.

## EMERSON HALL CONSTRUCTION UPDATE

Update by Jan McSherry, Chemistry Dept.

Work on Cherry Logan Emerson Hall is continuing on all levels. Installation of the elevator is complete. Mechanical, electrical and plumbing rough-in is continuing on all floors. The installation of the casework and lab equipment is continuing on all floors. The drywall is complete at the fourth floor and progressing at the fifth floor. Installation of the suspended ceiling grid is progressing at the first, second, third, and fourth floors. Exterior stucco application is progressing in all areas. Installation of the clay tile roof is complete. The completion date remains November 17, 2000, with 90% of the contract time completed as of Sept. 7.



Point your browser to <http://pm.fmd.emory.edu/emerson/emersoncam.htm> for live updates on the Emerson Hall construction and archives of previous pictures.

## NEW SENIOR ASSOCIATE DEAN TO OVERSEE EC OPERATIONS

Professor Lanny Liebeskind, formerly Chair of the Chemistry Dept., had been appointed Senior Associate Dean for Science and Sponsored Research of Emory College. One of Prof. Liebeskind's duties as Associate Dean will be to liaise with University-wide science programs including the Emerson Center. The appointment starts in Fall 2000. The office of the Associate Dean will be in the new Cherry Logan Emerson Hall.

## Letters from Fellows

I appreciated very much the opportunity to be a visiting fellow at the Emerson Center. I gratefully acknowledge Prof. Morokuma for his kind invitation.



Dr. Xin Lu

Especially I would like to thank Prof. Lin for recommending me and hosting my 9-month visit, which brought me the chance to meet with and learn a great deal from some active, prominent scientists. During my stay here, I have been working

intensively on the following topics: i) Calculation of Potential Energy Surfaces and Rate Constants for Some Combustion Related Reactions; ii) Quantum Chemical Study of the Chemisorption of Some Small Molecules ( $\text{NO}$ ,  $\text{O}_2$ ,  $\text{H}_2\text{S}$  and  $\text{SO}_2$  etc.) on Ideal and Defective Rutile  $\text{TiO}_2(110)$ .

It is the unreserved help from the Emerson staffs and the high-performance computational facilities available in the Center that made my stay enjoyable and fruitful.

*\*Dr. Xin Lu was a Visiting Fellow collaborating with Prof. M. C. Lin, one of the Emerson Center subscribers. He stayed at the Emerson Center from August 1999-April 2000.*

I would like to thank the Emerson Center for giving me a chance to spend four months in the group of Prof. Joel Bowman. I really enjoyed being at the Emerson Center. I found excellent computational facilities, very nice and enthusiastic people who enabled me to work on such exciting projects such as quantum molecular dynamics.

I wish to express my deep gratitude to Prof. Bowman for his guidance, encouragement and sharing of his time, knowledge and experience in creative discussions during the progress of my work. I was also very pleased that I had a chance to take his course CHEM 731, which provided me with the theoretical background of my project. My thanks also goes to his postdoc, Dr. Sergei Skokov, for his constant willingness to help. I also had stimulating scientific discussions with members of other groups. I really enjoyed group meetings, "Journals clubs" and many interesting seminars at the Chemistry Department. I appreciate also the excellent housing facility provided by the Emerson Center in the beautiful neighborhood on Clifton Road. It was a very nice place to live and relax after work. Finally I would like to thank the remaining members of the Emerson center for being so helpful and making my stay unforgettable.



Dr. Martina Bittererova

*\*Dr. Bittererova is Asst. Professor of Physical Chemistry at Slovak Technical University, Slovak Republic. She stayed at the Emerson Center as a Visiting Fellow from January to April 2000.*

## EMERSON CENTER VISITING FELLOWSHIP AWARDS FOR 2000-2001

Dr. Snezhana M. Bakalova, Bulgarian Academy of Sciences, Bulgaria

Dr. Stuart Carter, Univ. of Reading, United Kingdom

Prof. Ruben H. Contreras, Univ. Buenos Aires, Argentina

Prof. Sonia V. Ilieva, Univ. of Sofia, Bulgaria

Prof. Guan-Zhi Ju, Nanjing University, P. R. China

Prof. Jose Kaneti, Bulgarian Academy of Sciences, Bulgaria

Prof. Teerakiat Kerdcharoen, Mahidol University, Thailand

Prof. Steven H. Norton, State Univ. of West Georgia, USA

Prof. Ilkay Oren, University of Ankara, Turkey

Prof. Udo Schnupf, Troy State University, USA

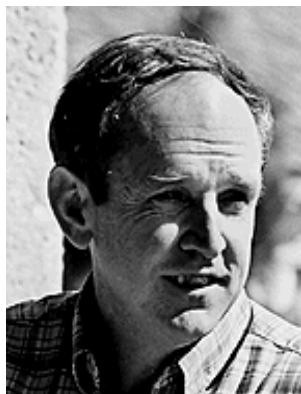
Prof. Lawrence M. Pratt, Fisk University, USA

*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, or send email to [clec@euch4e.chem.emory.edu](mailto:clec@euch4e.chem.emory.edu).*

## My Sabbatical at the Emerson Center

*Prof. William H. Miller, University of California-Berkeley*

My sabbatical this past spring in the Emerson Center was incredibly pleasant (as well as being scientifically fruitful). I would like to thank everyone at Emory for helping to make it so, especially Keiji Morokuma and Joel Bowman, and of course Jianli for taking care of all my practical questions, and most especially Cherry Emerson for providing the resources to make the entire program of the Emerson Center such a first class operation. As we begin to set up the Pitzer Center for Theoretical Chemistry here at Berkeley, the Emerson Center is a role model for what we hope to accomplish.



Prof. Bill Miller

In addition to having good experimental, as well as theoretical colleagues to talk with, I particularly enjoyed the chance to have hours of uninterrupted time to sit and do algebra!—it was like being a graduate student again. In fact, I worked through a very tedious and involved semiclassical (analytic) calculation that it is very unlikely I would have ever had the time to do otherwise. (For the experts, this is a continuous way of 'tuning' between a single and double phase space average in the initial value representation of a time correlation function; look for it in J Chem Phys later this year!)

It was also a very interesting visit personally, as a native Southerner being back somewhat on home territory. For example, I was able to see the gravesite of my 4th great-grandfather, John Miller, near Rutherfordton, North Carolina, as well as that of my (and also Maynard Jackson's!) 3rd great-grandfather, Robert McAfee (near the Holcomb Bridge over the Chattahoochee River). I had a very interesting and pleasant visit with Maynard Jackson with regard to this latter connection. So my semester at Emory was most educational in many ways!

## News from the Executive Committee Meeting

*The Emerson Center Executive Committee (ECEC) met on Sept. 7, 2000. EC Director Prof. Keiji Morokuma reported to the committee on administrative issues related to EC membership, 1999-2000 income and expenses, 2000-2001 budget, and summary of EC third staff position applications. The Center's technical staff presented to the committee members summary on their meetings with various vendors related to the EC computer system upgrade. The ECEC also reviewed applications to the EC staff position and proposed to invite one of the applicants for an interview.*



# Report on Research Activities at the Emerson Center

The Emerson Center is supported, in part, by "subscribers" -- faculty members or research groups who purchase shares in order to gain access to its resources for their research projects. The following are research activity reports from two subscribing groups of the Emerson Center.

## Kinetic of Epitaxial Thin Film Growth

Research Report by Prof. Fereydoon Family  
Department of Physics, Emory Univ.

Molecular-Beam-Epitaxy (MBE) is one of the most effective techniques for growing high purity materials including a variety of semiconductors and magnetic materials for applications in electronic and optoelectronic devices. In this method a constant flux of atoms impinge under ultrahigh vacuum conditions on a substrate held at a fixed temperature to grow a high quality crystalline material. The long-standing scientific challenge in this area has been to model epitaxial growth conditions and understand what are the fundamental processes that control the evolution of epitaxial structure and morphology.

Professor Family's research group in collaboration with Professor Jacques G. Amar of the Department of

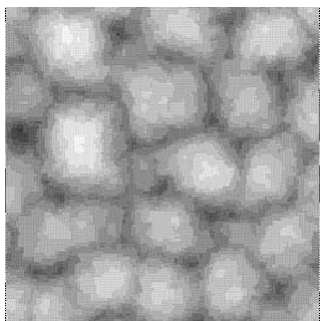


Fig. 1(a)

Physics and Astronomy, the University of Toledo, have used the resources of the Emerson Center to carry out large-scale kinetic Monte Carlo simulations of epitaxial growth as well as numerically solve self-consistent rate equations for irreversible island growth. One of the important topics studied is an experimentally observed instability known as "mound formation". Recently, it has been shown experimentally that even in the absence of effects such as strain, the surface is unstable and growth leads to the formation of surface mounds. The origin of this instability has been typically believed to be caused by the existence of an energy barrier (sometimes called the Ehrlich-Schwoebel barrier) to adatom diffusion over steps. However, theoretical calculations that we have recently carried out predict that even in the absence of such a barrier, a mound instability may develop due to the existence of a short-range attraction of adatoms to nearby islands and ascending

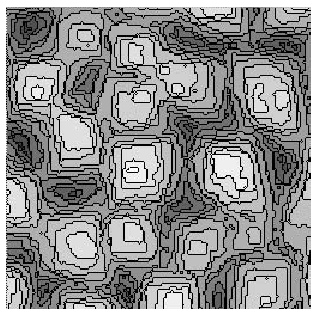


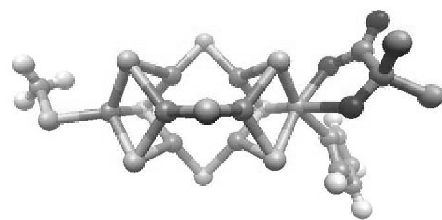
Fig. 1(b)

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## Computational Scientists Can Make a Difference

Research Report by Dr. Jamal Musaev  
Emerson Center, Emory Univ.

Recent developments in computer and software technologies have made computational chemistry one of the most promising areas of science. Today, computational chemists can effectively separate electronic and steric effects affecting the mechanisms of organometallic and bioinorganic processes, study the physical and chemical properties of large molecular systems with several thousand atoms, and predict new materials with given physical and chemical properties. Currently, my research at the Emerson Center involves the study of the mechanisms of 1) gas-phase reactions of bare transition metal cations and clusters with small molecules; 2) organometallic reactions, such as the transition metal catalyzed olefin polymerization,  $N\equiv N$  triple bond cleavage, alkene and alkyne hydro-, di-, thio- and sylla-boration, selective C-H and C-C bond activation; 3) reactions of small molecules with  $FeS_4$  and  $FeMoS_4$  clusters; 4) enzymatic reactions like hydrocarbon hydroxylation by methane monooxygenation (MMO), nitrogenase (nitrogen fixation on FeMo-cofactor; see scheme), and Fe-only hydrogenase; 5) problems related to the molecular wires and molecular scale electronics (computational approach to digital computing); and 6) reactions of small molecules on Si(100)-surface. In my research, I collaborate with Prof. K. Morokuma, Emerson Center director, EC subscribers Prof. M. C. Lin and Prof. K. Hagen, as well as Profs. C.C. Cummins (MIT), R.



Jordan (University of Chicago), T. Baker (Los-Alamos National Lab.), T. Marder (University of Durham, UK), M. D. Fryzuk (University of British Columbia, Canada), H. Basch (Bar Ilan University, Israel) and many others. For example, our collaboration with Prof. M. D. Fryzuk helped elucidate the structure of the  $[P_2N_2]Zr(m-h^2-N_2H)Zr[P_2N_2](m-H)$ , where  $[P_2N_2] = PhP(CH_2SiMe_2NSiMe_2CH_2)_2PPh$ , which previously (Fryzuk, M. D., *et. al. Science*, **1997**, 275, 1445), was incorrectly assigned as a complex with a dihydrogen ligand. Our calculations and latest neutron-diffraction experiments led to the same conclusion (see Basch, H.; Musaev, D. G.; Morokuma, K.; Fryzuk, M. D.; Love, J. B.; Seidel, W. W.; Albinati, A.; Koetzle, T. F.; Klooster, W. T.; Mason, S. A.; Eckert, J. J. *Am. Chem. Soc.* **1999**, 121, 523), and described this system as a compound with a  $Zr(\mu-\eta^2-N_2H)Zr(\mu-H)$  core.

Generally, in my research I follow the philosophy that dividing scientists into "computational" and "experimental" is incorrect, and a real scientist should be able to locate the important problems of science and solve them by all possible means, including computational. And, if necessary, one should collaborate with colleagues in attempts to solve the important problems of science.

## Want to Be a Subscriber?

The Emerson Center offers an introductory subscription of \$1250 per year, which gives the subscriber access to all Emerson Center research resources, both hardware and software, except for the privilege of hosting visiting fellows.

A no-cost 3-month trial subscription to the Emerson Center is also available for those who want to try out the benefit of subscription. For further information, please contact Dr. Musaev (7-2382, [musaev@euch4g.chem.emory.edu](mailto:musaev@euch4g.chem.emory.edu)) or Dr. Irle (7-4658, [sirle@emory.edu](mailto:sirle@emory.edu)) at the Emerson Center.

## Software Updates:

Lately, we have updated the quantum chemistry package GAMESS, have installed the Dalton program, and have implemented the Natural Bonds Analysis and NMR coupling constant programs into our widely used GAUSSIAN\_98 package.

The new version of the GAMESS (version May 2000) includes several new features among which I would like to emphasize the following:

- Vibrational Self-Consistent-Field (VSCF) method;
- Methods for evaluation of spin-orbit coupled constants;
- Methods evaluating analytic frequency dependent non-linear optical polarizability properties;
- Methods allowing to take into account the solvent effects, such as
  - a. effective fragment potentials (EFP)
  - b. polarizable continuum model (PCM)
  - c. conductor-like screening model (COSMO)
  - d. self-consistent reaction field (SCRF)

The Dalton\_1.0.1 program allows you to calculate the molecular properties based on SCF, MP2 and MCSCF reference wavefunctions. Using this program you can calculate:

- Geometries and transition states,
- Frequencies,
- Electric properties (Dipole, Quadruple moments, nuclear quadruple coupling constants, polarizabilities),
- Magnetic properties ( magnetizabilities, nuclear shielding constants, rotational g tensor, nuclear spin-rotation constants, spin-spin coupling constants, hyperfine coupling tensors),
- Optical and Raman properties (Vibrational Circular Dichroism, electronic Circular Dichroism, electronic adsorption, Raman Optical Activity).

*Jamal Musaev, Applications Software Manager*

### MOROKUMA ELECTED PRESIDENT OF IAQMS

*Professor Keiji Morokuma, Director of the Emerson Center, has recently been elected President of the International Academy of Quantum Molecular Sciences. He will serve a three-year term. The IAQMS is an organization of the top quantum molecular scientists in the world, and includes in its current membership 5 living Nobel prize winners. Said Dean Steven Sanderson of Morokuma's election, "It's a great honor, richly deserved."*

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

## Hardware Upgrades

### Tape Library Backup System Operational

The tape library backup system which the Emerson Center acquired a few months ago is now operational. It provides a more powerful backup solution compared to our old 8mm tape drives to protect the Center's software and, most importantly, protects user data from being destroyed, and guarantees data security. This tape library provides backup and random retrieval of up to 550 GB\* on 10 8mm DLT tape cassettes. Its backup speed of 6MB/sec. allows for rapid access to tape and thus enhances our data recovery service. Thus, the whole user space, currently 60 GB, is backed up within 6 hours, using 3 tapes. We create our weekly user data backup using this new device and keep the tapes for three consecutive weeks. In addition to this, we back up the entire system every other month. If a user loses data or accidentally removes files from his home directory, we will be glad to restore this data upon request, provided the data is on the tape. Please feel free to use this service.

*Stephan Irle, System Manager*

### A Note of THANKS from the Emerson Center

The Emerson Center staff would like to express our sincere appreciation to the Chemistry Department for their assistance in the previous issues of the Emerson Center newsletter and for their help to the Center in general. Our special thanks goes to Mrs. Sally Pete (formerly Sally Weeks) for her helpful suggestions for improving our newsletters and for help with proofreading.

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steps. Such an attraction has been observed experimentally in field-ion-microscopy observations of Ir adatoms near Ir clusters on the Ir(111) surface and is also supported by recent density-functional theory calculations.

In order to test our predictions, we have used the computers at the Emerson Center to carry out extensive simulations of the effects of short-range step-adatom interactions on both island nucleation in the early stages of growth and on the surface morphology in multilayer growth. Simulations of epitaxial growth on a bcc(100) surface were carried out for both the case of a short-range step-adatom attraction (Wang-Ehrlich effect) and well as in the case of step-adatom repulsion. The latter may occur in the case of epitaxial growth in the presence of surfactants.

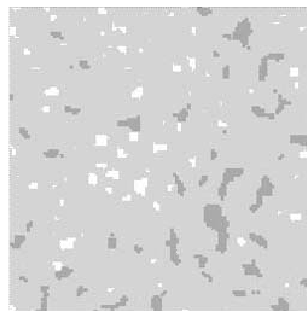


Fig.1(c)

As can be seen in Fig. 1(a) step-adatom attraction does lead to mound formation even in the absence of the Ehrlich-Schwoebel barrier to interlayer diffusion. In contrast, Fig. 1(b) shows that repulsion leads to smooth growth. In Fig. 1(c) we show the effects of competition between step barrier and repulsion. These findings have not only led to a deeper understanding of epitaxial growth, but also provide a practical tool for experimentalists enabling them to control the quality of surface using different materials or growth conditions.