EMERSON CENTER Newsletter

A Publication of the Cherry L. Emerson Center for Scientific Computation, Emory University
http://www.emerson.emory.edu
Volume 14, September 20, 2004

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News from the ECEC Meeting

The 18th meeting of the Emerson Center Executive Committee (ECEC) was held on Thursday, September 16, 2004. On the agenda were administrative issues, membership, technical reports, and the Emerson Center Lectureship Award Symposium. The committee also examined and discussed items on the balance and budget sheets of the Emerson Center operations account, approved the budget and the last of the four scheduled increases to the per share subscription fee, from $5775/year to $6000/year ($1500/year per unit). The current membership of the Center stands at 15.75 shares. Suggestions were made at the meeting regarding next years Lectureship Symposium and how attendance may be increased to involve more students. Prelimary meetings regarding the 2005 Lectureship Symposium will start in late September. Also discussed were issues related to scientific research activities of the center, and the initiative to write a proposal toward the Center's major computer upgrade. The scientific staff of the center reported on the upgrades to the Center's hardware equipment and software packages.

Emerson Center Symposium A Success

The first Emerson Center Lectureship Award Symposium, featuring the latest developments on the "Interface of Computers with Chemistry, Physics, Biology and Materials: Methods and Applications", concluded successfully on May 1, 2004. About 80 people, including faculty, students and postdocs from colleges and universities in Georgia, Alabama, and South Carolina attended this one-day event.

K. Morokuma, W. A. Goddard, and K. Warncke

In addition to the keynote speaker, Dr. William A. Goddard of Caltech, whose talk highlighted recent advances in theoretical and computational chemistry methodology, five other invited speakers gave talks on their respective area of research. Dr. S. Boettcher of Physics Dept., Emory University, considered the low-temperature properties of bond-diluted lattice spin glasses with up to $n=10^6$ spins, using an exact reduction method followed by the Extremal Optimization heuristic; Dr. R. Hernandez of Georgia Tech discussed the role of the environment in dense polymerization, protein motion and binding; Dr. J. Kindt of Chemistry Dept., Emory, talked about molecular and mesoscale modeling of membranes; Dr. J. Musaev of the Emerson Center analyzed the factors affecting the catalytic activity of transition metal complexes and proposed a new and more efficient catalyst for NN triple bond utilization built from first principles; and Dr. S. Stuart of Clemson University described the applications of bond-order potentials to a variety of problems, including hydrogen adsorption, sliding friction, and bond reorganization in carbon nanotubes, as well as energetic bombardment of polymers.

Prof. Lanny Liebeskind, Senior Associate Dean of Emory College, opened the event by welcoming all Symposium attendants and speakers, and expressed his gratitude to the Emerson Center Lectureship Award Selection Committee for their marvelous job in selecting excellent research topics and speakers for this Symposium. Dr. Donald Harris, Vice-Provost of Emory for Information Technology attended the special dinner honoring Prof. W. A. Goddard, winner of the 2004 Emerson Center Lectureship Award.

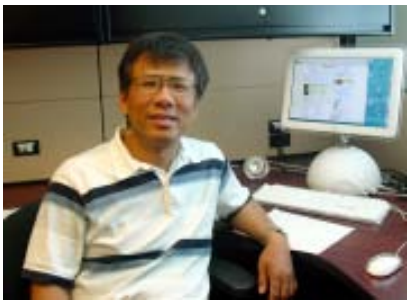
The EC Lectureship will be awarded annually and the award symposium next year is schedule for late April 2005 at Emory.

Emerson Center Welcomes New Subscriber

The Emerson Center welcomes Professor Jerry Thursby of the Economics Department of Emory University as a new subscriber to the Center. Professor Thursby's research interests lie in areas of econometrics and international trade and licensing of university technologies. He plans to use the Emerson Center resources in his research, and, in collaboration with Professor Mary Thursby at Georgia Tech, to take advantage of the Center's world-first implementation of the RIOTS_95 software combined with Matlab's Spline toolbox, allowing the handling of thousands of data points.

Letters from Fellows

After entering the door of the Emerson Center on the 5th floor of Emerson Hall to start my second summer visit to the Center, I immediately had the "not the same but still the same" kind of feeling about it. The Emerson Center is in fact now housed in a new building with new facilities, but I met again the same faculty and staff, and I rapidly understood that the Center is consistently working at the frontiers of knowledge. This lab offers researchers an opportunity to expand those frontiers in thriving on interdisciplinary research programs. In many current topics from atmospheric chemistry to biomolecules and nanomaterials, one could find someone here to have an in-depth discussion with. I enjoyed using both classical and electronic chemistry libraries. I have a good memory of the from-1-to-6-pm, intense and educational, seminars of Morokuma's group. I regret for not working this time with M.C. Lin's group due to his absence.



Dr. Ming Tho Nguyen at the EC

During my seven-week stay at the Emerson Center, I have investigated properties of different triradicals. The problem of three-electrons-in-three-orbitals is not only of fundamental interest in electronic structure theory, but also has applications in the emerging field of multi-spin materials. I have also looked at the blue-shifted hydrogen bonds, and thanks to the large computing powers, several novel blue-shifting complexes have been identified.

My family also enjoyed living in Atlanta and visiting the nearby regions. I look forward to pursuing this fruitful cooperation further.

Minh Tho Nguyen
Chemistry Professor
University of Leuven, Belgium

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Dr. Ming Tho Nguyen visited Emory as an Emerson Center Visiting Fellow from July to August 2004.

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 2005-summer 2006 is January 15, 2005. 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: January 15, 2005

My Stay at the Emerson Center as a Visiting Fellow

Ms. Biggi Albrecht, University of Oxford, UK

Some of you may already know me, but some of you may not, so allow me to introduce myself. My name is Biggi Albrecht and I have been at the Emerson Center since July. People often ask me where I am from, and the answer is not that simple. I do have a German passport, but I have lived in the UK for the last six years, so I guess that makes me European and probably also explains my German-London accent.

Back home I am in the final year of my PhD working with Prof. Graham Richards and Dr. Guy Grant at the University of Oxford (Brasenose College). My PhD thesis investigates new ways to model protein structures with special focus on reduced dimensionality representations. But when I heard about the Emerson Center and their visiting fellowships, I decided that it would be a good opportunity to learn more about membrane research, an area that has been in the back of my head since I was looking for interesting PhD projects.

I will be here until mid-October studying membranes with Prof. Kindt. We are particularly interested in the influence of curvature on membrane properties using molecular dynamics simulations to try to force straight bilayers into curved conformations and study their bending properties. Considering that I knew very little about bilayers when I first started and my knowledge of molecular dynamics was mostly theoretical, I realise how much I have learnt already. I hope that I can not only increase this knowledge over the remaining time, but also to make a meaningful contribution to my group's research.

Biggi in Atlanta

The Kindt group and of course Prof. Kindt himself have been incredibly helpful to get me started, and keep nudging me in the right direction. It has been a great honour and pleasure to work with them and to be invited to the Emerson Center for this summer. I have met many very talented bright people in the Emerson Center that have made me feel very welcome from the very first day. Even though I am still here I already regret that I will have to leave, but I wish everyone good luck and lots of success for their future projects.

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Ms. Biggi Albrecht is the first graduate student invited to the Emerson Center for collaboration research with an Emerson Center subscriber.

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.

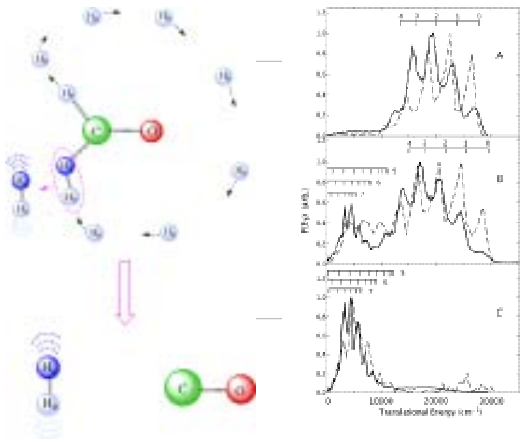
By-Passing the Transition State

Jaime Rheinecker, Xiubin Zhang & Joel M. Bowman

Department of Chemistry, Emory University

For two decades the mechanism of the dissociation of formaldehyde has left scientists scratching their heads. Although a mutually agreed upon mechanism has been established, lingering questions concerning the intermediate steps still inspire study after study to this day. It is known, for instance that H_2CO (S_0) + $h\nu \rightarrow H_2CO$ $(S_1,v,J,K_a,K_c) \rightarrow H_2CO$ $(S_0^*) \rightarrow H_2$ (v,J) + CO (v,J), yet it is unclear how the $S_1 \rightarrow S_0^*$ transition occurs. Is there a conical intersection? What about the presence of a triplet state? Does H + HCO play a role? These are some of the questions that we and Morokuma's group have either already addressed, or plan to in the near future.

In order to pursue these goals, postdoc Xiubin Zhang, together with Larry Harding at Argonne National Laboratory and former graduate student Shengli Zou, developed a new potential energy surface, the first one that describes both H_2+CO and the H + HCO channel. Xiubin and Jaime Rheinecker (third-year graduate student) have done dynamics simulations in parallel with new photodissociation experiments just completed by Arthur Suits' group. What we find is that at the energy of these experiments the molecular products are formed through a second, new channel that can best be described as a pre-H+HCO channel. This new channel, which completely bypasses the well-known saddle point for the molecular products, produces vibrationally excited H_2 and rotationally cold CO. This contrasts dramatically with the distributions found when the produts are formed via the well-known saddle point for these products. The very good agreement between theory and experiment on the correlated translational energy distributions (shown in the right-hand figure below) confirms the interpretation of a two-channel mechanism. We have made animations of trajectories that clearly show the two mechanisms. A graphic representation of one trajectory that "visits" the H+HCO channel before abstracting the H atom to form H_2 +CO is also shown above.



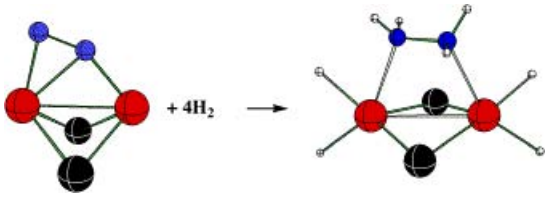
Thus, we have determined that formaldehyde has two mechanisms to make molecular products. We are now interested in H+HCO products. These products can also result from dissociation from the first triplet state. Together with Peng Zhang in Morokuma's group, who is mapping out the triplet surface, we plan to investigate the role the triplet pathway may play in the formation of these products.

Designing the Synthetic and Biological Catalysis from the First Principle.

Dr. Jamal Musaev, Emerson Center

Emory University

I am using the Emerson Center's facility, mainly, for the following research projects: (1) To elucidate mechanisms and factors controlling the extremely important chemical processes, such as transition metal-catalyzed nitrogen fixation, hydrocarbon oxidation, σ-bond (C-H and C-C) activation, alkene/alkyne boration, and olefin polymerization; (2) The application of the Nano-structures in the Catalysis (biological and non-biological) and the designing of new and more efficient catalysts; (3) The understanding of the important enzymatic processes such as oxygenase (for example, methanemonooxygenase) and nitrogenase;



(4) Cubane (Fe_nS_n, Fe_4Se_n, Fe_3MoS_4 etc) chemistry, involving electron transfer processes in the biological environment, and (5) A search for the effective drugs against peroxynitrite toxicity, and Se-based anti-cancer drugs (including bioactivation of chemopreventive Selenocysteine Se-Conjugates and Seleno metabolism)

For example, recently, I have demonstrated that the Zr_2Pt_2 cluster designed from the first principle, can easily react with dinitrogen and four dihydrogen molecules to produce hydrazine. The reaction starts from the coordination of the N_2 molecule to the Zr-centers of the Zr_2Pt_2 cluster. The resulting complex $Zr_2Pt_2(\mu\text{-}1,2\text{-}N_2)$ sequentially activates four dihydrogen molecules and produces the $(\mu\text{-}1\text{-}H)_2ZrPt(\mu\text{-}1,2\text{-}N_2H_4)PtZr(\mu\text{-}1\text{-}H)_2$ complex. Although the cluster Zr_2Pt_2 is designed to validate ideas on N_2 reduction by H_2 molecules, I believed that these findings might initiate new experimental approaches to study N_2 reduction by H_2 molecules by utilizing the advanced nanotechnology tools and the "cooperative" action of the multiple transition metal centers.

Recent EC Software Upgrades & New Software

Stephan Irle, Emerson Center

To accomodate the special requests of one new subscriber of the Center, the scientific staff of the EC has recently assisted in porting the **RIOTS_95** Matlab toolbox for solving optimal control problems (http://www.accesscom.com/~adam/RIOTS) to AIX. Until then, only Windows PC platforms were supported. Making RIOTS available on the UNIX platform has the advantage that future Linux and MacOSX implementations should be straightforward, increasing the reach of this toolbox to groups with powerful Linux Beowulf clusters. In order to run RIOTS_95 under Matlab, it was necessary to also install the **Spline toolbox** from Matlab, which has found immediate use in applications of the Physics Department subscriber group as well. These recent software additions demonstrate the increasing demand for modular mathematical program packages such as Matlab or Mathematica, which are now occupying EC CPU cycles in the 10-20% range, increasing fast. These program packages are more targeted at a broader user base, and we hope that embracing such software and growing in-house expertise will stimulate a greater outreach of the Center to the Emory scientific computational community.

In addition, we upgraded several quantum chemistry program packages. For instance, **GAUSSIAN** was upgraded to its latest version 2003 Revision C.1. The new features with respect to older versions are listed online at http://www.gaussian.com/g_tech/g03_rel.htm#newfeat and highlights are, e.g., new DFT functionals, performance improvements, and addition of more informative error messages. In addition, **GAMESS** and **NWChem** program packages were upgraded to their latest versions as well. **CPMD (**version 3.7.2) was installed for the first time, allowing to perform Car-Parinello-type quantum chemical molecular dynamics (QM/MD), as we noticed considerable increase in the popularity of QM/MD approaches with thus far more stationary-point-oriented theoretical chemists.

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

Installation of Powerbackup for EC's Main Servers

While Power Backup solutions are plentiful on the market place, it is fairly difficult to install reliable devices that actually work in the unexpected case of an emergency. After researching and shopping around, we found that a solution provided by APS with 5000 W provided the most competitive performance in reliability for the EC's main user login and mailing servers euch4e and its backup server. The surge protection and power backup unit is designed to provide power for about 1 hour, before automatic shutdown can be performed, protecting user data and environment from unexpected loss and eliminating painful restoration efforts.

Space Available at EC Apartment

The Emerson Center apartment on Clairmont Campus will have some vacancies in the winter and we would like to make it available to other short-term visiting faculty on campus. The apartment is fully furnished with cable TV and internet access. The rent, which includes all utilities and local telephone service, is $715 per room per month, or $40 per day if less than 30 days. Please call 727-0867 or email jzhao@emory.edu for more information.

EC Lectureship Symposium Speakers, left to right, S. Boettcher,, R. Hernandez, J. Kindt, J. Musaev

From left to right, S. Stuart speaks, award for W. A. Goddard, Emory Vice Provost Don Harris meets with participants, symposium reception