EMERSON CENTER Newsletter

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In This Issue . . .

What's New?

▲Starting March 19, 1999, the Emerson Center will offer a special series of **short courses on Practical Computational Chemistry**, taught jointly by the center's staff members, Dr. Jamal Musaev and Dr. Stephan Irle. For contents and schedule details, please refer to the announcement insert.

▲The Emerson Center is in the process of upgrading its **Main File Server** to meet the needs of the new and upgraded SP2, and to improve speed and users access. Details on page 3.

▲**Gaussian-98** and **Molpro-98** quantum chemical packages are now available at the Emerson Center's software collections. Please refer to page 4 of the newsletter for details about the above software packages.

MATH/COMP SCIENCES JUMP ON TRIAL SUBSCRIPTION

As part of our efforts to reach out to the broader Emory community, the Emerson Center Executive Committee implemented a free 3-month trial subscription to the EC facilities and software in the sping of 1998. This policy encourages and enables research groups from other departments on campus to try the Emerson Center services. After a visit to the EC Open House in September last year, Visiting Professor Paul Gray from the Math/Computer Sciences Department signed up for this unique opportunity. Prof. Gray's research areas include distributed computing and numerical partial differential equations, where standard parallel libraries like MPI are used. His major interest in this trial subscription is to find out whether our newly purchased SP2 can offer a good performance for his program code, written mainly in C++ and Java.

In order to accommodate "trial subscriptions", the Emerson Center has added a new subscribing group named "Trial" along with the regular subscribers, with adequate disk space and CPU time. In addition, a public domain version of the MPI parallel library and a (free)

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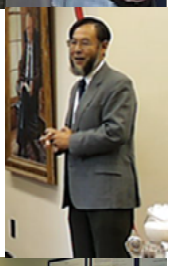
SECURITY ISSUES AT THE EMERSON CENTER

Due to an increased number of incidents of internet account break-ins, security of the computer system at the Emerson Center has become a major concern. The following is an excerpt from a recent memo by Marc Theune, software support for the Chemistry Department: "In recent days, hackers have been compromising the dooley accounts of people within or affiliated with the Chemistry Department. The hackers gain access to a person's login ID and password and begin to use the compromised account to cause trouble else-

-Continued on page. 4.

Scenes from the Open House

The Emerson Center held an open house on Friday, Sept. 11, 1998 to celebrate the major purchase of a new hardware system and the system software upgrade. Provost Rebecca Chopp spoke at the ceremony praising the achievement of the Emerson Center in promoting high-end scientific computation at Emory and its fellowship program hosting visiting scientists from all over the world.



Provost Chopp & EC Director Morokuma speaking at the Open House

Letters from Fellows

I appreciated the opportunity to spend a portion of my research leave at the Emerson Center. My 3-month stay in Atlanta was both productive and pleasant. The scientific and computational environment enabled me to initiate several projects during this time and to complete others.

Specifically, in collaboration with Prof. Keiji Morokuma, I carried out a series of benchmark calculations to further explore the application of ONIOM. In a second study, I explored the applicability of "chemical accuracy" methods such as G2 and G2M to the description of the stability of weakly bound molecular aggregates. A third project began the investigation of the structure and stability of a series of rhodium containing molecules that have potential as imaging agents when prepared with a radioactive isotope of Rh.

Prof. Patricia Plummer

The interaction with on-site Center subscribers, Profs. Heaven, Bowman, and Family, and other visitors to the Center and to Prof. Morokuma's group was intellectually stimulating and greatly added to the benefit of my time there. These scientists, together with the Emerson Center staff contributed significantly to my stay. Special thanks are due to Stephan, Jamal and Dima for "putting up" with my many questions and requests—especially in the beginning.

In summary, the Cherry Emerson Center and its director Prof. Morokuma provide an environment which is very supportive and in which a visitor can be scientifically productive.

**Dr. Patricia Plummer is Professor of Chemistry and Physics at the University of Missouri, Columbia, Missori. She stayed at the Emerson Center as a Visiting Fellow from September to December 1998, and is scheduled to visit the center again in March 1999.*

1999-2000 Visiting Fellowship Announcement

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, physics, and other sciences for one to several months are encouraged to apply. We also accept faculty on sabbatical leave. Postdoctoral research associates are not supported through this program. Travel expenses (and stipends for long term stays) are available. Although fully independent research is not excluded, collaboration with an EC subscriber is desirable, and EC subscribers are encouraged to make recommendations.

To formally apply, please submit:
- *1-2 page research proposal,*
- *CV including publication list,*
- *the amount of financial support needed and*
- *the length of stay and an approximate start/end date*

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

DEADLINE TO APPLY IS
FEBRUARY 1, 1999

Upgrading my Research at the Emerson Center

Prof. Yoshihiro Osamura, Rikkyo University, Japan

I am very much appreciative to Prof. Keiji Morokuma for giving me a chance to spend my sabbatical year at the Emerson Center. I was amazed that only a few people are maintaining such a good facility and nice research environment for computational chemistry. The leadership and aggressive research activities here at the Emerson Center are owing to not only people gathered here but also to the support from Dr. Cherry Emerson and Emory University. The wide range of research field in computational chemistry carried out here inspires me a lot during my stay. This means that many researchers who are interested in computational chemistry can become involved in research here, e.g., from excited state dynamics of atom and diatomics to biological systems as well as catalytic processes. Such a fascinating place made it possible for me to extend my research interests.

Prof. Yoshihiro Osamura

I was able to make major progress on my research about analyzing the interaction of hydrated clusters of strong acids, reaction mechanism of [2+2] cycloaddition reaction of benzyne, formation mechanisms of interstellar molecules, and the development of full variational methods to optimize electronic wavefunction and molecular geometry simultaneously.

**Prof. Osamura is a Visiting Fellow at the Emerson Center from April 1998 to March 1999.*

The Emerson Center Apartment

The Emerson Center has a long-term lease for a fully furnished 2-bedroom apartment for its visiting fellows. The apartment is a well-maintained, independent carriage house located at 1223 Clifton Road, less than 5 minutes walk to campus. It is ideal for short-term visitors since it is fully furnished with full-size beds in each bedroom, linen and sheets, kitchen utensils, and couches and oriental rugs in the living room.

We make the apartment available to other short-term visiting faculty on campus when there is a vacancy. The rent, which includes all utilities and local telephone service, is $550 per room per month, or $25 per day if less than 30 days. Please contact Jianli Zhao at 727-0867 for more information.

Report on Research Activities from EC Subscribers

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.

Energy Transfer in Lasers

Prof. Michael Heaven
Department of Chemistry

Electronic energy transfer and the formation of molecules in metastable electronic states are the targets of our recent computational efforts. This effort is motivated by the need to understand energy transport and transfer in chemical laser systems. High-power iodine lasers depend on energy transfer from singlet oxygen to atomic iodine. We have examined this process by computing potential energy surfaces that represent the forces acting between I and O_2 in various electronic states. Our results explain the magnitude of the transfer cross section and its dependence on temperature. This study also demonstrates that electronic structure methods have now advanced to the point where reliable results can be obtained for problems of this kind.

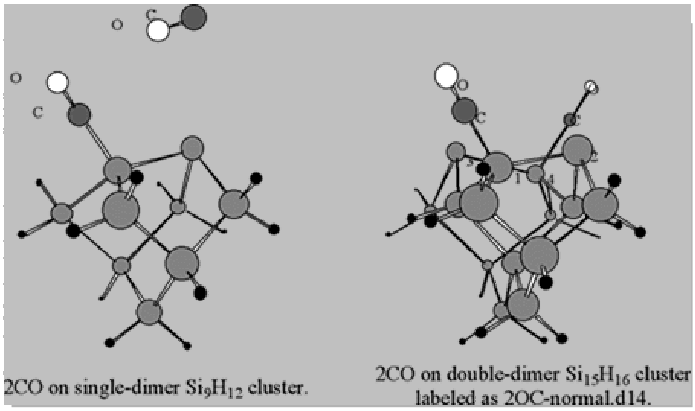
Efforts are currently under way to use singlet NCl (isoelectronic with O_2) to drive iodine lasers. Following our success with $I+O_2$, we are computing potential energy surfaces for I+NCl. Among other issues, we want to know if energy transfer in this system occurs by a purely physical exchange, or if transient formation of a chemically bound INCl intermediate is involved. Ultimately, this question determines the mechanism of heat release in the laser.

These are technically challenging problems, as they involve electronically excited states and relativistic effects must be included. As this is not routine quantum chemistry, we are grateful for Prof. Morokuma's participation in this collaborative venture.

A Model Study of "CO-CO Adsorbate Interaction" on Si(100)-2x1

A Report from Prof. M.C. Lin's Laboratory
Department of Chemistry

The CO-CO adsorbate interaction on Si(100)-2x1 has been investigated with *ab initio* molecular orbital and hybrid density functional theory calculations using cluster models of the surface. Different adsorption combinations for one and two CO molecules on single- and double-dimer cluster models, Si_9H_{12} and $Si_{15}H_{16}$, respectively, are used. Our calculations indicate that the second CO molecule is physisorbed on the same surface Si dimer where the first CO molecule is chemisorbed. The chemisorption of the first CO molecule induces a change in the charge of the surface Si dimer atoms which inhibits further adsorbate-dangling bond interaction. This greatly reduces the ability of the surface to accept an additional CO molecule on the same Si dimer. The dissociation energy of the physisorbed second CO molecule is less than 1 kcal/mol. Adsorption of the second CO molecule on the second Si dimer is energetically favored for the 2OC-normal.d14 structure as the most stable configuration, with the two CO molecules adsorbed diagonally across the two Si dimers. The dissociation energy of the chemisorbed second CO molecule in the 2OC-normal.d14 structure is 13.9 kcal/mol. Inter-configuration, i.e. OC-normal and OC-bridge, interaction between CO adsorbates have also been studied. The adsorbed CO is found to be more stable in the OC-normal than the OC-bridge configuration. At the B3LYP/6-31G(d) level of theory, our calculations predict that the OC-normal could not coexist with the OC-bridge configuration on adjacent surface Si dimers.



2CO on single-dimer Si_9H_{12} cluster. 2CO on double-dimer $Si_{15}H_{16}$ cluster labeled as 2OC-normal.d14.

EC File Server Upgrade

The Emerson Center is in the process of upgrading its main file server to meet the needs of the new and upgraded SP2. This upgrade to a modern IBM server model based on IBM's new POWER3 technology will enable users to access their home directories and programs during computation, increase access speed to NFS mounted disks, and dramatically increase the Emerson Center computation facility's total storage capacity. An option will be available so that the SP2 nodes can mount file systems from the file server over the "SP Switch", SP2's forty-times faster network.

Want to Be a Subscriber?

Take Advantage of the 3-month Free Trial & the Introductory Subscription Offers

At the recent Emerson Center Executive Committee meeting, an introductory subscription of $1250 per year was approved . This low-cost introductory subscription offers 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 still 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) or Dr. Irle (7-4658, sirle@emory.edu) at the Emerson Center.

Software:

Gaussian-98 & Molpro-98
now available at the Emerson Center

Gaussian-98 is the latest in the Gaussian series of electronic structure programs. It is designed to model a broad range of molecular systems under a variety of conditions. Gaussian-98 can predict the energies, molecular structures, vibrational frequencies and numerous molecular properties for systems in gas phase and in solution, and it can model both their ground state and excited states. Users with experimental backgrounds can use this program to study molecules and reactions of definite or potential interest, including both stable species and those compounds which are difficult or impossible to observe experimentally (short-lived intermediates and so on).

Gaussian-98 includes many features specially designed to bring large molecular systems within reach of electronic structure methods. Advanced optimization algorithms and other efficiency innovations make semi-empirical geometry optimizations practical for larger molecules than ever before.

Fast multipole method (FMM) and sparse matrix techniques for linearizing computational cost and an enhanced integration algorithm substantially extend the practical range of DFT calculations, especially for frequency calculations.

The ONIOM facility in Gaussian-98 brings this powerful method of Morokuma and coworkers to Gaussian users. Using this technique, which divides a molecular system into two or three "layers" which are treated at different levels of accuracy, very large molecules of biological and commercial interest become feasible for study. ONIOM allows, for example, the active site of a drug molecule to be modeled using a very accurate model chemistry, while atoms close to it are treated at a somewhat lower level of theory, and atoms far from the site are treated in a more approximate manner. ONIOM calculations in Gaussian-98 may use any of the available methods for the various layers defined for a molecular system currently under investigation.

Gaussian-98 continues to extend the range of molecular properties that can be predicted. NMR shielding tensors and chemical shifts can be computed at the MP2, HF and DFT levels. Vibrational circular dichroism (VCD) intensities may be predicted at the HF and DFT levels. Raman intensities may be predicted using DFT and MP2 methods in addition to HF.

The ZINDO semi-empirical method is available for studying the excited states of very large molecules. The CI-Singles method remains Gaussian-98's first-level ab initio facility for modeling excited states. Gaussian-98 can also predict excited state energies via time-dependent methods (TD). These calculations may be carried out at the HF and DFT methods.

We also recommend to our users another powerful electronic structure package, Molpro-98, which is extremely efficient for study of excited states of small molecules (up to 10 atoms). This package is available at our Center, and will be described in detail in our next newspaper.

Jamal Musaev, Applications Software Manager

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

***Gray/EC collaboration**, continued from page. 1*

native Java compiler from IBM have been installed. Regular production jobs for existing subscribers are not affected. It can even be expected that specific needs for existing subscribers with their own program development may benefit from parallelism technologies brought in by researchers like Prof. Gray. This exchange of knowledge will eventually improve communication between all of the EC users.

Prof. Paul Gray is current running his first set of tests on our SP2 computers. We feel that the Emerson Center has benefited from this experience. We have learned from knowledge that other research groups from different backgrounds have brought to us. Finally, we would like to take the opportunity and encourage other potential users to take advantage of the trial subscription to try out the center's most advanced facilities.

For information about the free subscription offer, please refer to our web site at: http://www.emerson.emory.edu/local/free-subs.html.

PLEASE VISIT US AT OUR WEB PAGE:

http://www.emerson.emory.edu

The Emerson Center web page gives the most up-to-date information about the Emerson Center operations. You will have access to information about the center's Mission Statement, the current list of the centers subscribers and their research interests, updates about our Visiting Fellows Program, software and hardware upgrade information, news on conferences and other programs that the center initiates, tutorials, and links to many other exciting sites.

***Security issues**, continued from page. 1*

where on the internet. The electronic trail of the troublemaking then leads back to the user's compromised account. . . . Usually, the hackers use our accounts to disrupt internet relay chat rooms or usenet groups. However, it is possible ... that our account will be used in attempts to break into sensitive governmental systems."

To the best of our knowledge, the EC was not involved in these attacks. But in order to monitor the security of our system, we installed a password-guessing program on Oct. 29. This program was able to guess a huge number of user passwords within just 1 minute, which means that many EC accounts were essentially open for anybody in the world. Since Friday, Dec. 11 we have successfully enforced the use of good passwords for all our EC users. A good password contains:

- *8 characters*
- *upper & lowercase letters*
- *numbers and special characters*

We realize that any password can easily be cracked by installing so-called "network sniffer programs" somewhere on the network. These programs monitor login processes to any computer on the internet and read login ID and passwords in clear text if used by a user over the internet (rlogin procedures, telnet). An encryption mechanism would be required to close this security hole, and all EC computers can now be reached using ssh (Secure Shell) which implements this kind of password encryption. We strongly encourage everybody to use 'ssh' in the future, which can be obtained without charge for UNIX machines at http://www.cs.hu.fi/ssh, and for $50/license for PC's and Mac's at http://www.datafellows.com.

Stephan Irle, System Manager