EMERSON CENTER Newsletter

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◆ MOROKUMA TO RETIRE FROM EMERSON CENTER

Prof. Keiji Morokuma, William H. Emerson Professor of Chemistry and Director of the Emerson Center, announced his retirement from both the Chaired Professorship and Emerson Center Director position effective August 31, 2006. Dr. Morokuma has served as the Emerson Center Director since 1993 and has played a key role in bringing the center to its prominent international recognition today. Much has been accomplished during Dr. Morokuma's directorship, including establishing Emory as one of the world's centers for computational science, while providing world-class computing power for Emory's scientific computational community. The establishment of the Center's Visiting Fellowship Program and the EC Lectureship Award Symposium series has also contributed to promoting interaction and collaboration between computational scientists at Emory and those from all parts of the world. We appreciate Prof. Morokuma's 13-year service to the Emerson Center and Emory University and wish him "Happy Retirement!" (although Dr. Morokuma will continue his research at Emory after retirement and we understand his research group will remain active for the near future).

KARPLUS SELECTED FOR 2006 EC LECTURESHIP AWARD

The third annual Emerson Center Lectureship Award Symposium, featuring the latest developments on "Computational and Mathematical Modeling in Large Systems: From Proteins to Cells", will be held on April 3, 2006, in White Hall Room 207. The 2006 award winner is Professor Martin Karplus of Harvard University (USA) and ISIS Université Louis Pasteur (France). Professor Karplus is considered an icon in the field of computational and mathematical modeling of biological systems. He will present a keynote speech on "How Proteins Work: Insights from Simulations" at the symposium.

In addition to Professor Karplus, several other leading scholars will also give talks at the symposium. They include Emory professors Dieter Jaeger of Biology, David Lynn of Chemistry and Biology, and Kurt Warncke of the Physics Department. Professor Steve Harvey of the School of Biology, Georgia Tech, and Professor Ying Xu of Biochemistry and Molecular Biology, the University of Georgia, are also invited to speak at the symposium on the latest developments in their laboratories.

Prof. Martin Karplus

Students and postdocs are encouraged to participate and present their latest research results during the poster sessions and compete for the two "Best Poster" Awards.

Invitations are sent to faculty, students and postdocs of colleges and universities in Georgia, Alabama and South Carolina and between 100-120 participants are expected to attend this one-day event. In additional to our previous sponsors (Gaussian, IBM, Mitsubishi Chemical and Sun Microsystems), James River Technical and the Coca-Cola Company are added to our symposium sponsor list. Please refer to the Emerson Center website for details and the up-to-date symposium information: http://www.emerson.emory.edu/conferences/index.html.

EC CONTINUES INT'L COLLABORATION

The Emerson Center continues to expand international collaboration in computational materials science. During its 14 years of existence, the Center has established itself as one of the foremost points of contacts when it comes to setting up and conducting collaborative research projects in the area of computational sciences, thanks mainly to its ingenious visiting fellowship program, but also to its increased visibility by means of the recently established Emerson Center Lectureship Award Symposium and the active research conducted by its scientific staff. Following Dr. Jamal Musaev's fruitful visit to the University of Tokyo in the summer of 2002, a recent visit of Dr. Stephan Irle to Japan and Korea on a JSPS Short Term Visiting Fellowship as coordinator of the Emory computational nanomaterials research team of the Morokuma Group helped to significantly promote Emerson Center's position among Japanese and Korean scientists.

Dr. Irle's main goal during his 6-week stay at Nagoya University at the lab of Prof. Hisanori Shinohara, a world-famous metallofullerene and peapod chemist, was to establish close contacts between the Shinohara research team and to

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Letters from Fellows

I visited Emerson Center as a Visiting Fellow in November-December 2005. Prof. Keiji Morokuma was so kind to invite me to make some investigations of hydrogen adsorption at carbon nanostructures. It was the first time I visited Emerson Center and generally United States for scientific research. I was

Dr. Alexander S. Fedorov

very surprised that it was so convenient to work in the Center: powerful computers, very comfortable conditions of work, even at night, good facilities for search of new scientific information promoted to work. Even possibilities for sport exercises were great!

Though I did not have experience of working with Mac and AIX-based computers before, after some days of hard work and especially thanks to invaluable help of Dr. Stephan Irle, I was able to run tasks already.

I am very thankful to Prof. Morokuma as well as Drs. Stephan Irle and Jamal Musaev for guidance and fruitful discussions. And I would like to thank Jianli Zhao who helped me in many important official affairs.

So, after my short visit of the Emerson Center I often remember this warm (in both meaning) place and the colleagues in the Morokuma group. And I dream that I will visit the Center again in the not distant future.

Dr. Alexander S. Fedorov
L.V. Kirensky Institute of Physics
Krasnoyarsk, Russia

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Dr. Alexander S. Fedorov visited Emory as an Emerson Center Visiting Fellow from Nov. 15 to Dec. 15, 2005.

Emerson Center Visiting Fellowship Awards for 2006-2007

Dr. Valentin P. Ananikov, Russian Academy of Sciences, RUSSIA
Dr. Michael B. Darkhovskii, Karpov Institute of Physics, RUSSIA
Dr. Juan Elezgaray, CNRS, UMR, FRANCE
Dr. Stefan Heldmann, University of Lubeck, GERMANY
Dr. P. Kolandaivel, Bharathiar University, INDIA
Dr. Hsin-Yi Liao, National Taipei University of Education, TAIWAN
Dr. Stephan Mertens, Otto-von-Guericke University, GERMANY
Dr. Seiji Mori, Ibaraki University, JAPAN
Dr. Maxim A. Olshanskii, Moscow M. V. Lomonosov State Univ., RUSSIA
Dr. David Quinonero-Santiago, Univ. de les Illes Balears, SPAIN
Dr. Amit Raj Sharma, Max-Planck-Institut fur Plasmaphysik, GERMANY
Dr. Paolo Sibani, Fysisk Institut, SDU, DENMARK
Dr. John Rui-Hua Xie, Hubei University, P. R. CHINA

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. Jee-Gong Chang, Associate Researcher & Electro-Optical Leader, NCHC, Taiwan

I was thrilled to receive the opportunity to visit the Emerson Center, Emory University, as a Visiting Fellow from March to September last year. I thoroughly enjoyed staying at the apartment kindly arranged for me by the Emerson Center on Clairmont Campus, with its tranquil and beautiful surroundings and first-rate athletic facilities. I explored the campus thoroughly and particularly enjoyed sampling the extensive range of delicious food available both on campus and in the neighborhood.

Dr. Chang attended the 6th Int'l Conference on Chemical Kinetics during his EC visit.

My goal in visiting Emory was to advance my knowledge of large-scale quantum chemistry computation in the gas and solid phase chemistry reaction kinetics field. Thanks to the guidance and instruction I received from Prof. M. C. Lin during my stay I am now able to make a significantly greater contribution to the ongoing success of Taiwan High Performance Computing Center here in Taiwan. Emory provides an excellent research environment with outstanding hardware and software resources. Furthermore, the many academic seminars, conferences and group meetings held during my time there were of great personal interest and benefit to me.

I miss the green grass and warm sunshine of Atlanta very much. It is no exaggeration to say that living and studying at Emory University was truly a joy for me.

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Dr. Chang spent 6 months at the Emerson Center as a Visiting Fellow, from March to September 2005, collaborating with EC subscriber, Prof. M. C. Lin's research group.

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.

Prediction of Kinetics and Mechanism for ClO_x Gas-phase Chemistry and Ammonium Perchlorate (AP) Related Condensed Phase Chemistry

R. S. Zhu and M. C. Lin
Department of Chemistry, Emory University

A. ClO_x gas-phase chemistry

Over 60 elementary reactions of AP and the formation of its early decomposition products from NH_x to ClO_y (x = 2, 3; y = 0 - 4) have been investigated in great details. The detailed potential energy surfaces and T, P-dependent rate constants have been supplied, many of which are directly relevant to the chemistry of the Freon-polluted stratosphere for which no such detailed theoretical calculations existed in the literature. Key results have been reported in a recent review chapter [*R. S. Zhu and M. C. Lin, a book chapter on Energetic Materials, Part 2, Detonation and Combustion, P. Politzer and J. S. Murray, eds. chp. 11, pp. 373 - 443, Elsevier Science Pub., 2003.*]

B. Elucidation of the condensed phase chemistry

The sublimation of NH_4Cl has been successfully modeled quantum mechanically by VASP (Vienna Ab-initio Simulation Package). The supercells containing 2 x 2 x 2 (including 8 mono-NH_4Cl cells) and 3 x 3 x 3 (27 mono-NH_4Cl cells) were used in the calculations. The result supports the heretofore unexplained experimental finding that the activation energy for the sublimation process is lower than the enthalpic change and that the molecular complex of NH_3 and HCl desorbs concurrently as a pair. The selected energy diagram for 2 x 2 x 2 model is plotted in Fig. 1.

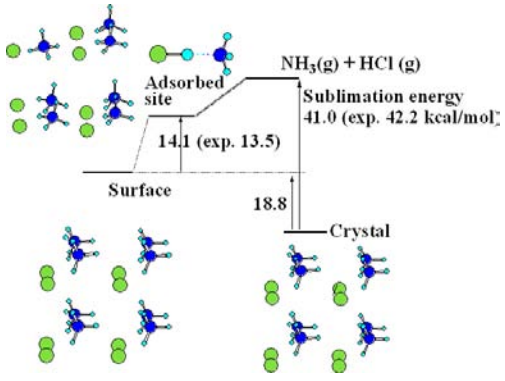
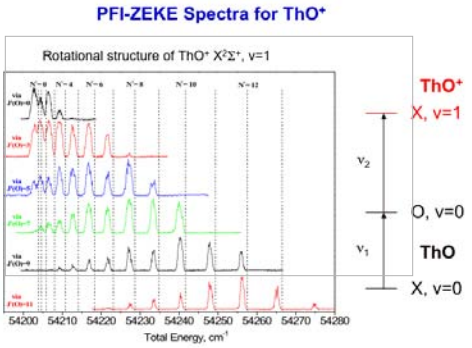


Fig.1. Sublimation (dissociation) energy diagram for a 2 x 2 x 2 model of NH_4Cl, calculated by VASP

Spectroscopic evaluation of relativistic quantum chemistry calculations

Michael C. Heaven
Department of Chemistry, Emory University

Experimental studies of actinide compounds that contain short-lived or radioactive isotopes are expensive and hazardous. Consequently, efforts are underway to develop computational methods that are capable of making reliable predictions of the properties of actinide compounds. The goal is to develop relativistic quantum chemical methods that will provide capabilities for modeling heavy-element compounds similar to those currently available for light-elements. High-level theoretical models of the electronic structures and properties of actinide compounds are currently being developed by several research groups. This is a challenging problem due to the need for explicit treatment of relativistic effects, and the circumstance that many of these molecules exist in states where the *f* and/or *d* orbitals are partially filled. The latest generation of theoretical models must be tested and evaluated through comparisons with experimental results. Gas phase data are most suitable for this purpose, but there have been very few gas phase studies of actinide compounds. In the present project we are carrying out gas phase spectroscopic studies of simple Uranium and Thorium compounds (oxides and halides). To complement the experimental effort we are also investigating the potential for using relativistic *ab initio* calculations and empirically adjusted Ligand Field Theory models to predict and interpret the electronic energy level patterns.



Uranium dioxide is a molecule that exemplifies the theoretical and experimental challenges presented by actinide compounds. There have been conflicting predictions of the ground electronic configuration and a troublingly large and persistent difference between the calculated and measured values for the first ionization energy (IE). We recently characterized UO_2 using resonant multi-photon ionization techniques. The IE was found to be 0.7 eV higher than the previous experimental values, but in excellent agreement with the predictions of a large CASPT2 calculation (with explicit treatment of the spin-orbit interaction). The CASPT2 ground state was also consistent with the experimentally determined configuration. Further relativistic calculations are being used to assign the electronic spectra of UO_2. Experiments on thorium monoxide show that ionization weakens the metal oxide bond, while reducing the equilibrium bond length and increasing the vibrational frequency (examples of the spectra for ThO^+ are shown in the figure). The latter trends are usually associated with an *increase* in the bond strength. DFT calculations that used relativistic core potentials successfully reproduced these contradictory characteristics. These results indicate that significant progress is being made with relativistic quantum chemistry methods, but many challenges remain. Our work indicates that more efficient ways to treat intershell electron correlations are needed, among other improvements.

EC Hardware/Software Report

Drs. Jamal Musaev & Stephan Irle, Emerson Center

◆ **Beefing Up Security at the EC**

Following the recommendations and with the help of the College's ITD Technical Support Team (many thanks to Derek Spransy and Todd Sirmans), the Emerson Center has considerably increased the barrier of its already tough to crack AIX and Linux machines. A deplorable incident, during which the insufficiently secure password of one EC user was cracked in late September last year, caused one of our computers to be hacked and made to attack other computers on the Emory network. Luckily, we were able to stop these illegal activities quickly and close the vulnerable account. This incident shows how important it is to maintain secure passwords, and as a consequence of this incidence and other recent increased computer breakins at the the Chemistry Department, we are no longer permitting weak passwords. From 9/23/05, all new user passwords have to conform to the following standard:

- 8 character in length
- 1 non-alphanumeric (special) character such as *,#,!

In general, passwords should not be guessable, they should not contain your spouse's name, pet's name, etc... One good way to make a fool-proof password is to take a sentence and use the first letters of each word with different capitalization. For instance:

"My cat has a nice black hat" - McHa!nBh

We have already turned on enforcement of these secure password characteristics on euch4e and users with insecure passwords are automatically notified by our own password cracker. In addition, we have closed a number of ports not necessarily needed, although we are keeping ftp and telnet protocols open as a service to mainly international visiting fellows.

◆ **Installation of Additional software on Fire**

We have continued to install additional software on Fire, which includes the following software packages: parallel GROMACS 3.2.1, parallel VASP 4.2.6, parallel AMBER 8, parallel OpenMX 2.73, sequential GAMESS 03, and an experimental sequential version of the deMon software 1.1.0 which contains a DFTB package implemented by Thomas Heine and Dennis Salahub. The fire Linux cluster has become even more popular among our subscribers and we are hoping that these recent software additions will be beneficial to our user base. Behind the scenes, but very important for a smooth operation of our integrated platform combination of AIX and Linux computers, shell scripts have been developed and improved that guarantee a very smooth interface between IBM's LoadLeveler and the underlying OpenPBS queueing system software on Fire.

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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 $710 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 Int'l Collaboration, continued from page 1.

initiate promising research projects. The Morokuma/Irle/Shinohara collaborative team currently has six projects that are actively progressing, in almost all cases employing quantum chemical molecular dynamics simulations (QM/MD) and standard ab initio density functional theory and related calculations, a methodology which has been successfully developed at the Emerson Center to unravel the mystery of fullerene formation. In addition, the Morokuma/Irle team is now actively collaborating with the Japan Fine Ceramics Center in Nagoya, where in a promising new experimental approach, chirality specific carbon nanotubes are formed by thermal treatment of SiC crystals.

Two weeks traveling to 12 experimental and theoretical research groups in Japan (from Sendai to Hiroshima) have broadened Dr. Irle's horizon for the incredibly busy research activities in Japan in the area of computational nanomaterial's science, opened possibilities for new collaborations, and affirmed his love and admiration for this truly remarkable country, its culture, and the people.

Report from the ECEC Meeting

The Emerson Center Executive Committee (ECEC) met on Friday, February 10, 2006 for its 21st meeting. Present were committee members R. Antia, G. Hentschel, D. Lynn, K. Morokuma, V. Sunderam, and K. Wilkinson, as well as Emerson Center staff members. On the agenda were administrative report, technical report, lectureship symposium, and the selection of the 2006-2007 Emerson Center Visiting Fellowship Awards. Out of about 30+ applications received, the 2006-2007 EC Visiting Fellowships were awarded to 13 scientists and scholars residing in regions including China, Denmark, France, Germany, India, Japan, Russia, Spain and Taiwan (list on page 2). The scientific staff members of the Center reported on the current updates on the Center's hardware and software conditions, including the enhancement of the Center's system security in collaboration with ITD staff members. Reports were also presented on the progress of the 2006 Emerson Center Lectureship Symposium, and the re-submission of EC's major equipment funding proposal to NSF. Prof. Morokuma announced to the committee his retirement at the end of the current academic year.