

Chemistry Alumni Newsletter
University of North Dakota
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Current Faculty

Analytical:	David Pierce, Julia Zhao
Chemical Ed:	Julie Abrahamson, Tom Ballintine
Inorganic:	Harmon Abrahamson, Ewan Delbridge, Lothar Stahl
Organic:	Anamitro Banerjee, Alexei Novikov, Irina Smoliakova
Physical:	Mark Hoffmann, Jenya Kozliak, Kathryn Thomasson
Adjunct:	Eric Murphy, Leroy Pazderny, Matthew Picklo

Barry Carpenter 2005 Abbott Lecturer



Barry K. Carpenter was born in Hastings, England, in 1949. He received a B.Sc. (1st class honors) in Molecular Sciences from Warwick University (1970) and a Ph.D. in Organic Chemistry from University College London (1973). During 1973-75 he was a NATO Postdoctoral Research Fellow in Yale University. He joined the Chemistry Department at Cornell University in 1975 and has been a Professor since 1985, serving as Department Chairman from 2001 to 2004 and becoming the Horace White Professor of Chemistry and Chemical Biology in 2004.

Professor Carpenter's research uses a combination of theory and experiment to study fundamental questions of reaction mechanism. On the theoretical side, his research group uses *ab initio* electronic-structure calculations and quasiclassical molecular dynamics simulations. The experimental work involves organic synthesis, followed by kinetics studies, some

of which are carried out in supercritical fluids.

Professor Carpenter is a member of the American Chemical Society, the American Association for the Advancement of Science and the Royal Society of Chemistry (London). His awards include the Alexander von Humboldt Senior Scientist Award (1990), the Stephen & Margery Russell Teaching Award (1992), the ACS Arthur Cope Scholar Award (1997), and the ACS James Flack Norris Award in Physical Organic Chemistry (1999). Professor Carpenter has been an Alfred P. Sloan Research Foundation Fellow (1980-82), a John Simon Guggenheim Memorial Foundation Fellow (1986), and is a Fellow of the American Association for Advancement of Science. He has been an Associate Editor or a member of the Editorial Advisory Board of several journals: *Journal of the American Chemical Society*, *Accounts of Chemical Research*, *Journal of Organic Chemistry*, and *Organic and Biomolecular Chemistry*. He is an author of a book, several book chapters and more than 100 papers.

Lecture April 21

Teaching and Learning Science

This talk will review the ways that science is currently being taught and learned, both inside the classroom and out, and will present the speaker's personal opinions about the aspects of the enterprise that work well and those that could be improved. Some effort will be made to discuss the broader implications of ensuring scientific literacy for a large fraction of the population.

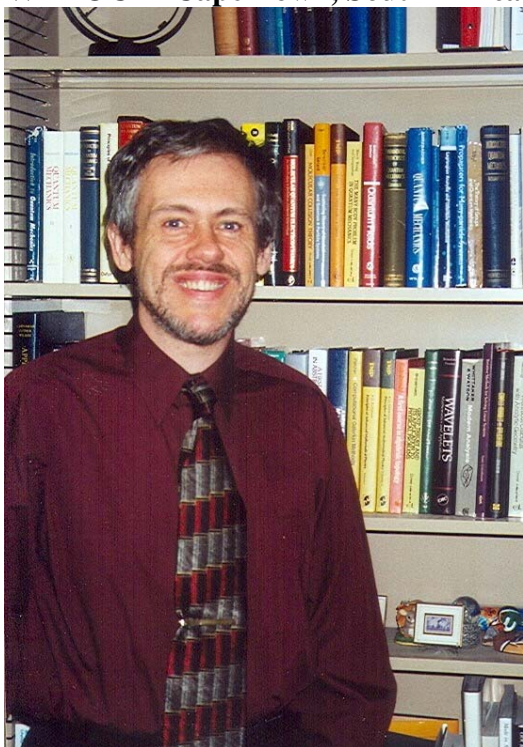
Lecture April 22

Nonstatistical Dynamics in Thermal Reactions of Polyatomic Molecules

Starting in the 1930s, the theoretical models of reaction kinetics that form the basis for our current understanding of reaction mechanisms began to be developed. An important approximation that went into two of the principal theories – RRKM theory and Transition State Theory – is now being revisited and found to be less generally applicable than originally believed. The so-called statistical approximation assumes that the excess (primarily vibrational) energy in molecules undergoing thermal reactions can be treated as always statistically distributed among the available modes. It implies that intramolecular vibrational energy redistribution (IVR) must always be faster than any bond-breaking or –making event.

Work in the speaker's laboratory, and others, now seems to be showing that this assumption is not reliable. Its revision has profound implications for the description of reaction mechanisms. For example, it implies that the behavior of reactive intermediates is not necessarily independent of the way in which they are prepared, and that reactions occurring via achiral intermediates do not necessarily have to give racemic products.

Mark Hoffmann Gives Invited Presentation at the 7th Congress of the WATOC in Cape Town, South Africa



The meeting marking the 7th official congress of WATOC (World Association of Theoretical and Computational Chemists, formerly known as World Association of Theoretically Oriented Chemists) took place on 16 – 21 January 2005 in Cape Town, South Africa. The conference theme was “**Modeling Structure and Reactivity**”, and a number of internationally renowned speakers, including Mark Hoffmann of UND, delivered talks. Hoffmann's talk, which was based on work that he and Dr. Yury G. Khait, Hoffmann's research associate at UND since 1997, performed, was titled “**Generalized Van Vleck Multireference Perturbation Theory for Molecular Electronic Structure.**” The talk high-lighted their recent progress on a second-order, multiconfigurational, multireference perturbation method for molecular electronic structure, based on Generalized Van Vleck Perturbation Theory (GVVPT2). GVVPT2 is both state-selective and of the “perturb-then-diagonalize” type of multireference perturbation theory. GVVPT2 is capable of a balanced treatment of nondynamic and dynamic electron

correlation for even very challenging systems, while requiring only a relatively modest $O(n^5)$ scaling of computational effort. The revised GVVPT2 actively uses the recently introduced concept of macroconfigurations, which allows arbitrarily complex incomplete model spaces to be used efficiently. Exploiting the capability of using large one-electron active spaces, the method has even been applied to problematic excited electronic states of unsaturated, highly strained ring systems, such as CF_2O_2 and CF_2N_2 , and to the hitherto debated ground state of Co_2 .

Hoffmann's work on multireference perturbation theory was previously supported by the National Science Foundation (1999–2003) and is currently supported by a grant from the Department of Energy (2004–2007), which emphasizes developing the method for use in high-performance computing environments.

Mark Hoffmann Gives Computational Chemistry Workshop at the University of Buea, Cameroon, Africa

Mark Hoffmann was invited to lead a computational chemistry workshop at the University of Buea, Cameroon, which he presented with the assistance of his graduate student, Alexander Azenkeng. The workshop emphasized the use of techniques of modern quantum chemistry for the understanding of the structure and energetics of molecules, with particular emphasis placed on organic molecules. As opposed to presenting the techniques in a purely “blackbox” framework, each technique was preceded by lecture material on the underlying theory. The workshop was held on 10 – 14 January, with morning sessions emphasizing theory and afternoon sessions providing “hands-on” experience with simple, but non-trivial problems. Approximately 20 students attended, and faculty from Buea and as far away the universities in Yaoundé and Dschang took the opportunity of sitting in on one or more topics. UND Chemistry has accepted, as incoming graduate students, two students who attended the workshop in January. There are prospects of collaborations between faculties, and already a manuscript is in preparation that has Hoffmann and the chemistry department chair of University of Buea, Dr. Mac Thomas Akam, as co-authors.

In addition to financial support from the University of Buea, the workshop would not have been possible without the generous support of many offices at UND, including those of President Charles Kupchella, Vice-

President Peter Alfonso, Vice President and Provost Martha Potvin, Graduate School Dean Joseph Benoit, and the UND Alumni Foundation.

UND Student Wins International Poster Prize



Alexander Azenkeng wins a Gold Best-in-Session Award at the 7th official congress of WATOC meeting. At this meeting, in addition to invited talks such as Dr. Hoffmann's, there were several contributing lectures and two poster sessions, with over 400 delegates from 48 different countries in attendance, and only a small percentage of these were students.

Alexander Azenkeng had the privilege to be one of these student-delegates and presented a poster on "**Multireference spin-adapted variant of density-functional theory and its implementation**". This is new theory that represents a significant development in density-functional theory approaches for addressing correctly problems that hitherto have been challenging for conventional methods. During the poster session, Alexander faced some tough questions from many of the renowned theoretical chemists that were in attendance. The end Alexander won one of the two overall best-in-session Gold awards. Alexander writes: "It was perhaps more exciting to meet many of the past and current Schrödinger and Dirac medalists and hear them speak, as well as meeting other well-known personalities in this field. Besides learning how to deliver a talk at a meeting of this magnitude, there was certainly a lot of inspiration to be drawn from these people."

Julia Zhao Wins SACP Award



Development of Novel Fluorescent Nanosensors for Rapid, Sensitive and Selective Determination of Selenium in Organic Matte: The emerging field of nanotechnology promises to provide revolutionary tools for chemical analysis, including that of selenium. The applicant proposes to take advantage of the nanoparticle for this sensor since nanoparticle provides a high surface to volume ratio and a high fluorescence signal. This combination of properties will provide a much higher sensitivity, as well as a rapid and simple detection of target materials (in this case selenium) compared to traditional methods.

SCAP is The Society for Analytical Chemists of Pittsburgh, a non-profit organization dedicated to the advancement of analytical chemistry through science education. Website: <http://www.sacp.org/>

Kathryn Thomasson Elected to National Council of Prestigious Women's Science Organization

On June 11, Kathryn Thomasson was elected to the National Council of IΣΠ, the National Honor Society for Women in Chemistry. Dr. Thomasson was elected to the post of Director of Student Awards because of her efforts to encourage women in Chemistry and her service to the Members at Large of IΣΠ; for the previous two triennia she has been serving as Coordinator for Members-at-Large.

IΣΠ is a national honor society for women, which promotes professional development and personal growth of women in chemistry and related fields through recognition, public outreach, and the formation of supportive networks. For information about membership qualifications or about the undergraduate or graduate student awards, please contact K. Thomasson at kthomasson@chem.und.edu. IΣΠ website: <http://www.iotasigmapi.info/>.

Please Join Us for Homecoming!

On Friday Sept 30 we will have our Alumni Lecture, Student Award Ceremony and Banquet. Please join us. For more information please contact Tom Ballintine, tballintine@chem.und.edu.

Alumni News

Dawn Wellman writes: I recently completed my PhD in chemistry from Washington State University and am a staff scientist for the Department of Energy at the Pacific Northwest National Laboratory in Richland, WA - better know as the Hanford Site, most noted for the contribution to the Manhattan Project. I've conducted so many projects that I decided it best to simply include my CV to describe what I've been working on. However, in a nutshell it could most aptly be boiled done to aqueous and solid phase uranium geochemistry and the development of nanoporous metal phosphate materials to sequester aqueous heavy metal and radionuclide contaminants. I've also attached the link for our groups website if you're interested in finding out more about

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what we do here - largely environmental remediation for DOE and DOD.

Rajeev and Hina Pandey announces the birth of their daughter Raeva on November 7, 2004.



Felix Ngassa took his first students to the National ACS meeting in San Diego in March. Two of his students presented research posters.

Return Service Requested