Chemistry Alumni Newsletter
University of North Dakota
Spring 2004
Volume I Number 2

Current Faculty by Division

Analytical (David Pierce); Chemical Education (Julie Abrahamson, Tom Ballintine); Inorganic (Harmon Abrahamson, Ewan Delbridge, Lothar Stahl); Organic (Anamitro Banerjee, Bill Shay, Irina Smoliakova); Physical (Mark Hoffmann, Jenya Kozliak, Kathryn Thomasson).

A Message from the Department Chair, Mark Hoffmann

Greetings, friends! It is my privilege to serve as Chair during these exciting times in UND Chemistry. The Department is expanding both its research productivity and its educational impact. Last year we reported for the first time in recent years $1M in new research funding, which arose from 7 grants; 8 of 11 tenure-track faculty members had publications; we were successful in hiring two additional very well qualified faculty; there are 73 undergraduate majors and 29 graduate students. The new Biochemistry option of the Chemistry degree promises to engage additional majors. Long-time friends of the Department will see that there are many new faces, but the traditions and spirit of UND Chemistry are alive and well. Please enjoy this newsletter and especially accept my personal invitation to join us for this year's Abbott Lectures.

Abbott Lectures: April 29 & 30
138 Abbott Hall

Speaker
William H. Miller
Department of Chemistry
University of California Berkeley

William H. Miller received a B.S. in Chemistry from Georgia Tech (1963) and a Ph.D. in Chemical Physics from Harvard (1967). During 1967-69 he was a Junior Fellow in Harvard's Society of Fellows, the first year of which was spent as a NATO postdoctoral fellow at the Physikalisches Institute of Freiburg University (Germany). He joined the chemistry department of the University of California, Berkeley, in 1969 and has been Professor since 1974, serving as Department Chairman from 1989 to 1993 and becoming the Kenneth S. Pitzer Distinguished Professor in 1999.

Professor Miller's research has dealt with essentially all aspects of molecular collision theory and chemical reaction dynamics. Most recently his efforts have focused on developing the initial value representation (IVR) of semiclassical theory into a practical way of adding quantum effects to classical molecular dynamics simulations of chemical processes.

Professor Miller is a member of the International Academy of Quantum Molecular Sciences (1985), the National Academy of Sciences (1987), and the American Academy of Arts and Sciences (1993). His awards include the Annual Prize of the International Academy of Quantum Molecular Sciences (1974), the E. O. Lawrence Memorial Award (1985), the Irving Langmuir Award in Chemical Physics (1990), the American Chemical Society Award in Theoretical Chemistry (1994), the Hirschfelder Prize in Theoretical Chemistry (1996), the Ira Remsen Award (1997), the Spiers Medal of the Royal Society of Chemistry (1998), and the Peter Debye Award in Physical Chemistry (2003).

Lecture 1: April 29, 7 PM, Room 101
Abbott Hall, UND

Using Semiclassical Theory to Include Quantum Effects in Classical Molecular Dynamics Simulations. Semiclassical (SC) theory provides a good description of essentially all quantum effects (interference/coherence, tunneling, symmetry effects of identical particles, quantization of bounded motion, etc.) in molecular dynamics; this has been long appreciated and validated by many applications to small molecular systems [cf. *Adv. Chem. Phys.* **25**, 69-177 (1974)]. Since SC theory is built on the classical trajectories of the dynamical system, it should in principle be possible to use it also to add quantum effects to classical molecular dynamics simulations of *complex* molecular systems (i.e., those with many degrees of freedom), e.g., chemical reactions in solution, in clusters, in bio-molecular or

any complex environment. The practical implementation of SC theory for systems with many degrees of freedom is based on various initial value representations (IVRs), which have recently undergone a re-birth of interest in this regard. This talk reviews the basic idea of the SC-IVR approach and describes a variety of recent applications that hat been carried out using it. [For a recent overview, see *J. Phys. Chem. A* **105**, 2942-2955 (2001).]

Lecture 2: April 30, 12:00 Noon, 138 Abbott Hall, UND

The Quantum Instanton Approximation for Thermal Rate Constants of Chemical Reactions. A quantum mechanical theory for chemical reaction rates has recently been developed [*J. Chem. Phys.* **119**, 1329 (2003)] which is a generalization of the earlier semiclassical (SC) instanton approximation [*J. Chem. Phys.* **62**, 1899 (1975)]. This *quantum instanton* (QI) description has many of the qualitatively desirable features of the earlier SC model--e.g., the reaction rate is expressed wholly in terms of the Boltzmann operator of the system--but it corrects its major quantitative deficiencies by utilizing the *quantum* Boltzmann operator, exp(-*H*/kT), rather than its SC approximation. Since calculation of the quantum Boltzmann operator is feasible for quite complex molecular systems (by Monte Carlo path integral methods), having an accurate rate theory that involves only the Boltzmann operator could be quite useful. Application of the QI approximation to several one- and two-dimensional model problems illustrates its potential; e.g., it is able to describe thermal rate constants accurately (no more than ~10-20% error) from high to low temperatures deep into the tunneling regime, equally well for asymmetric as well as symmetric potentials. A recent application to the H + CH_4 → H_2 + CH_3 reaction in its full (18d) cartesian space (using Montel Carlo path integral methods) illustrates how the approach can be implemented for reactions involving many degrees of freedom.

Announcing the Hiring of Two New Faculty in Chemistry

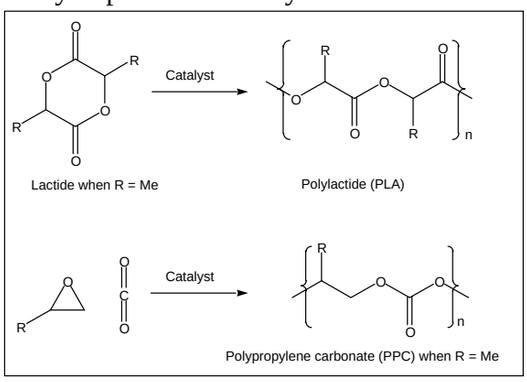
Beginning this fall, two new faculty will join the department as assistant professors. Dr. Julia Zhao is an analytical chemist with interest in making nanoparticles for remote sensing particularly for biomedical applications. Her projects include the design, synthesis and characterization of novel nanoparticles for biomedical & biotechnological applications, rapid and ultrasensitive bacteria/virus testing paper based on nanoparticle-molecular beacon probes, and flow DNA microchip using fluorescent nanoparticle probes. Dr. Alexei Novikov is a synthetic organic chemist with interest in natural product synthesis. His projects include remote functionalization and synthesis of germacronolides.

Introducing Our Newest Faculty Member Ewan Delbridge, Inorganic Chemistry

Ewan Delbridge joined the Chemistry faculty this past fall as an assistant professor. He received his B.Sc. (Hons. 1st Class) in 1995 at Monash University, Australia. Ewan then went on to complete his Ph.D. in 1999 also at Monash University, Australia under the direction of Professor Glen B. Deacon in organolanthanide chemistry. After completion of his Ph.D., Ewan worked with Professor Malcolm H. Chisholm as a Postdoctoral Researcher from 2000-2003 at The Ohio State University. While at UND he is establishing his research and has already won the UND New Faculty Scholar Award. One research project is

Synthesis of Novel Schiff Base Lanthanide(III) Complexes as Catalyst Precursors for the Ring-Opening Polymerization of L-lactide. An explosive area of research is in the search for new polymers that are derived from renewable resources and are biocompatible or biodegradable. These will ultimately lead to the replacement of existing polymers that are currently derived from fossil fuels. Polylactide is derived from a renewable resource (corn starch) with large-scale commercialization already in production. This polymer shows great promise not only as a packaging material, but also in the medical industry as a drug delivery agent. Dr. Delbridge is synthesizing a series of lanthanide(III) complexes containing appropriate ligands that would make ideal catalysts for the ring-opening

polymerization of lactide. The impetus behind using lanthanide compounds as catalysts is that they offer distinct advantages over transition metal and main-group catalyst systems. The highly electropositive nature, coupled with the ionic contraction across the series of the lanthanide metals, makes them ideal candidates as systematic fine-tuning of the catalytic pocket is readily achieved.



Announcing the Newest Program in Chemistry: B.S. Major in Chemistry - Biochemistry Option

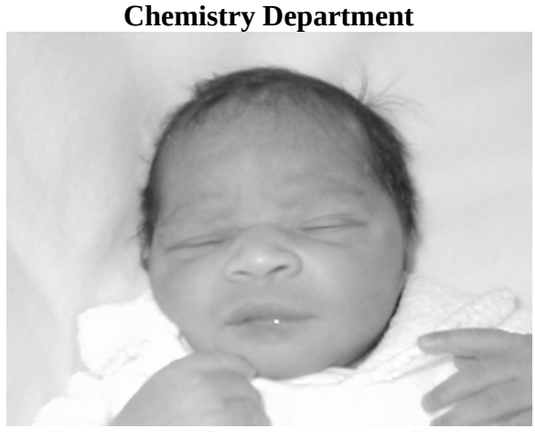
Thanks to support from the faculty in the Biochemistry & Molecular Biology Department in the School of Medicine and Health Sciences, this fall we are able to launch a new program in Biochemistry for which we will seek to have ACS certification. The new B.S. program is based on the successful B.S. with Major in Chemistry - Health Sciences Option. New courses have been added and the mathematics requirement increased from one semester of calculus to two.

Two new courses have been approved and will be through the Department of Biochemistry & Molecular Biology beginning this Fall. These courses build upon the current BMB 301, which is a prerequisite. This new option will provide a strong biochemistry background for students interested in varied pursuits, from the job market to graduate studies in chemistry, biochemistry, physiology, microbiology, and medical fields.

BMB 401. ***The Biochemistry of Proteins and Information Flow.*** 3 credits. This course will build upon the overview of biochemistry and molecular biology as presented in BMB 301. Lectures will emphasize advanced topics in protein structure and function, enzymology, and the expression and transmission of genetic information. An independent project in proteomics or computational biochemistry will be required. Fall Semester. Prerequisite: BMB 301.

BMB 403. ***Advanced Biochemistry Laboratory.*** 2 credits. Prerequisites: BMB 401 (may be taken at the same time) and permission of the instructor. Students will demonstrate competency in understanding and performing physical and molecular techniques commonly used in biomedical research. Fall Semester. Initially BMB 403 will be offered out of research labs in the department. Faculty have agreed to assume responsibility for providing mentoring, space and equipment necessary for students to become proficient in a specific technique. The goal is to establish an equipped teaching lab space in the College of Arts and Sciences would make it possible to offer BMB 403 to up to 30-40 students per semester, thus increasing the maximum capacity of the course and the degree program.

Welcome the Newest Member of the Chemistry Department



Favor Bongfen, daughter of Yvonne Bongfen, a first year graduate student in the Chemistry Department, was born on March 3, 2004 at 7:04 PM. Favor was 5lbs. 5.7ozs and 18 3/4 inches. She's busy growing now.

Julie Abrahamson Becomes Regular Faculty

Dr. Julie Abrahamson has taught freshman chemistry courses at UND since 1992. She was officially added to the chemistry faculty in August 2003 as assistant professor. Her primary teaching and course development responsibilities are in freshman courses for non-science and pre-nursing majors, Chem 115 and Chem 116. She is also critical to the development of the new B.S. Major in Chemistry - Biochemistry Option.

Alumni News

Shelia Lofthus Merschman writes: "I recently got the chemistry alumni newsletter. What a great idea! I would love to hear where all our alumni are now. I am working for Merck (a large pharmaceutical company) in West Point, PA. I got this job right out of school and have been here 6 years. I am still in the area of analytical chemistry working in clinical drug metabolism. I've even done some work on drugs you may have heard of like Vioxx and Fosamax. Oh, and on a personal note, I have a wonderful 18 month old daughter, Paige."

Felix Ngassa is now a tenure track assistant professor at Grand Valley State Univeristy where he is starting up his research with undergraduates.

Michelle (Ward) Muscatello writes: I was married (hence the name change) on October 4th to Aaron Muscatello who I have been seeing for a little over 4 years (on and off at times). I also graduated with my MS in August and am continuing on for the Ph.D. My MS was in Analytical Chemistry and the title of my thesis was "Development of an Intelligent Polymerized Crystalline Colloidal Array for in vivo Detection of Signature Cancer Proteins"

Coretta Fernandes shares the following, a link of the article in the Lansing State Newspaper about the Science Olympiad.
http://www.lsj.com/news/schools/040229_olympiad_1b-3b.html
Coretta organizes and holds this event at her college every year for high school and middle school kids. She has been interviewed for TV and the interview will be broadcast on MI cable TV.

Chemistry Alumni Newsletter
c/o Kathryn Thomasson, Editor
UND Department of Chemistry
PO Box 9024
Grand Forks, ND 58202-9024

3133-1905

Return Service Requested