

Curriculum Vitae Comments

General

With varying degrees of overlap, my career has focused on roughly three major phases, research (1965-1980), administration (1981-1987) and teaching (1987-2002). My style may be described as innovative, generalist and constructive.

Research

My research career began as a student at the University of Utah working under the direction of Henry Eyring. I had the distinction of being the first graduate student to use a high-level programming language (FORTRAN) on the first solid state computer (the IBM 1620). Soon after I arrived at the University of New Mexico, I began forming relationships with national laboratories, first as an Associated Rocky Mountain Universities Fellow at Los Alamos National Laboratory and later through visiting staff member appointments at LANL and Lawrence Laboratory Laboratory. I spent summers, semester breaks and a sabbatical leave at Laboratories in a variety of experimental and theoretical physics and chemistry groups. I participated in research projects with people like Ed Hammel, Fritz Schaefer, Charlie Bender, Arnold Karo, Berni Alder, John Sullivan and Don Thompson. During this period I directed three PhD students in theoretical chemistry. I did both analytical theory and computational theory employing supercomputers to perform calculations that would not have been possible in a local university environment of that time. Research was focused on molecular dynamics, quantum mechanics, liquid theory and kinetics.

My research mode was to usually publish a single paper of some significance in a given field. Thus, I was engaged in pioneering collaborative theoretical computations of molecular electronic structure and properties including: the first quantum mechanical calculation reproducing the observed geometry of water, the first calculation of the structure and bonding of an organic free radical intermediate (methylene), the first accurate calculation of van der Waals forces (revealing a weakly bound state of dihelium), the first full-dimensional variational calculation of the vibrational motion of a tetraatomic molecule (ammonia), a limited-CI quantum mechanical six-dimensional potential energy surface calculation of reactions associated with the HeH₃⁺ molecule, accurate at the "chemistry" level (0.1 kcal/mol), the first theoretical prediction of a dissociative charge transfer reaction (based on an accurate full-CI potential energy surface calculation of the six lowest states of the HeH₂⁺ molecule). Some of these theoretical calculations stimulated reinterpretation of experimental studies.

Administration

In 1983, I installed and managed the UNM Chemistry Department's first computer system, consisting of two DEC VAXes running Ultrix. A variety of software tools of interest to chemists (such as molecular structure and rendering programs, x-ray and nmr analysis, numerical utilities and publishing software) were installed and maintained. Beginning in 1966 I began writing an expanding suite of grade processing and maintenance programs (first in Fortran, then in C), used up until 1999 by numerous faculty teaching general chemistry laboratory and lecture. In 1994 I built and administered the UNM Chemistry Department's first web pages to deliver department and course information, student bulletin boards and faculty research interests.

Between 1981 and 1987 I served two terms as Director of the Los Alamos Graduate Center, an on-site learning facility contracted by the AEC with UNM. A number of novel developments took place during this appointment. Course offerings were extended in several science and engineering departments, an MBA program was developed and courses at the medical school were initiated. I wrote the first software at UNM to facilitate remote on-line course registration on main campus and used it to register students in Los Alamos. I participated in the development of the state's first distance conferencing and learning facility linking Los Alamos (Graduate Center and Laboratory) with Sandia National Laboratory, UNM and White Sands Missile Range. Two-way live video classes, seminars and meetings were conducted and, for the first time classes taught by experts at LANL were delivered to students at state universities.

In 2000 I organized the UNM Complexity Network, consisting of faculty members from five departments with interest in the emerging field of complexity science (<http://www.unm.edu/~plectics>). Its purpose is to promote courses, stimulate interaction and eventually develop a curriculum leading to degrees in a new profession.

Teaching

I have taught courses in each traditional division of chemistry (General, Analytic, Organic and Physical) and taught General Chemistry more than 30 times. I tend to never repeat the same material in a given course twice and have initiated new courses in a dozen areas, of which Chemistry 325 (Undergraduate Readings), 466 (Scientific Computation), Computer Science 131/132 (Introduction to Unix and the World Wide Web) and Computer Science 365 (Introduction to Scientific Modeling) have become regular offerings in the UNM curriculum. These courses tend to attract both undergraduate and graduate students from a wide variety of disciplines including science, engineering, economics and humanities. In 1988 I began writing programs to automate experimental analysis in general, analytical and physical chemistry lab courses, culminating in 1995 in complete web lab experiments containing descriptions, procedures, analysis, reports and video demos. I have written or am writing textbooks in General Chemistry, Physical Chemistry and Modeling, posted the first Internet chemistry textbook (1994) and am in the process of developing web-based versions of some of my courses. I have been nominated for outstanding teacher recognition six times and received the Alumni Association Faculty Award for 1999.

Don McLaughlin, July, 2002