



UNIVERSITY OF MINNESOTA
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Department of Chemistry

Bryce L. Crawford Lectureship

Professor Martin Gruebele

Department of Chemistry
University of Illinois at Urbana-Champaign

Website:

http://chemistry.illinois.edu/faculty/Martin_Gruebele.html

Faculty Host: Professor Laura Gagliardi

Professor Martin Gruebele received his bachelor's degree in 1984, and his doctorate in 1988 from the University of California at Berkeley. After working as a postdoctoral fellow at the California Institute of Technology, he joined the faculty of the University of Illinois in 1992. He also is a faculty member of the Beckman Institute.

The Gruebele Group is engaged in experiments and computational modeling to study a broad range of fundamental problems in chemical and biological physics. A common theme in these experiments is the implementation of state-of-the-art laser techniques to interrogate and manipulate complex molecular systems, coupled with quantum or classical simulations. The results of these efforts are contributing to a deeper understanding of the way that proteins fold into functional 3-dimensional molecules, the details of how chemical bonds are broken by vibrational motion and how this can be controlled, and the switching of energy flow in large molecular structures on surfaces.



Fast Folding Proteins Meet the Anton Supercomputer

9:45 a.m.

**Thursday, March 1
331 Smith Hall**

During the past 15 years, a number of small proteins (30-80 residues) have been engineered to fold particularly fast, even “downhill” (without a significant activation barrier). These model systems are ideal for comparison with molecular dynamics simulations, which have lengthened into the millisecond region, while experimental folding rates have been compressed to a few microseconds. Such overlap allows a direct comparison of rates, stability and mutational effects on folding mechanism. I will present examples of fast folding proteins, some examples of computer-experiment comparison during the last 10-15 years, leading up to the current state of the art in comparing experiment and simulation.

Bryce L. Crawford Jr. was a renowned Department of Chemistry professor and scientist. He died in September 2011, at the age of 96. He joined the department in 1940, and became a full professor of physical chemistry in 1946. He was chair of the department from 1955 to 1960, and was dean of the graduate school from 1960 to 1972. He retired in 1985. He loved studying molecular vibrations and force constants, and the experimental side of molecular spectroscopy and molecular structure. During World War II, Crawford worked in research on rocket propellants, making significant contributions to rocketry, and the development of solid propellants for the much larger rockets that evolved after the war. Crawford received many honors during his career, including the prestigious American Chemical Society Priestley Medal; and being named a Fellow of the Society for Applied Spectroscopy, a Guggenheim Fellow at the California Institute of Technology, and a Fulbright Fellow at Oxford University. He held the distinction of membership in three honorary science academies, and was actively involved in many professional associations.

