

September 2005

Chemistry Weekly, Volume 1 Issue 23, September 5 - 9, 2005

Follow this and additional works at: <http://digitalcommons.unl.edu/chemistryinfo>



Part of the [Chemistry Commons](#)

"Chemistry Weekly, Volume 1 Issue 23, September 5 - 9, 2005" (2005). *Department Information -- Chemistry*. 1.
<http://digitalcommons.unl.edu/chemistryinfo/1>

This Article is brought to you for free and open access by the Chemistry, Department of at DigitalCommons@University of Nebraska - Lincoln. It has been accepted for inclusion in Department Information -- Chemistry by an authorized administrator of DigitalCommons@University of Nebraska - Lincoln.



Special Interests:

New Chemistry Department Staff
UNL Service Awards, State of the University Address
And All University Picnic - Friday, September 9, 2005
EHS Colloquium - September 20, 2005

Volume 1 Issue 23

Monday, September 5, 2005 -
Friday, September 9, 2005

A WEEKLY PUBLICATION OF THE DEPARTMENT OF CHEMISTRY

Chemistry Weekly

COLLOQUIUM

Professor Bruce S. Hudson

PROFESSOR OF CHEMISTRY
BIOPHYSICAL CHEMISTRY AND CHEMICAL PHYSICS
SYRACUSE UNIVERSITY

*"Vibrations of Molecules in Solids: Periodic DFT
and Inelastic Neutron Scattering"*

Friday, September 9, 2005
3:30pm - Room 112 Hamilton Hall



Professor Bruce S. Hudson
Ph.D Harvard University 1972

My major current research area involves the application of vibrational inelastic neutron scattering and modern periodic Density Functional Calculations to problems involving the structure and dynamics of molecular crystals. We are also involved in a collaborative research project with the Borer Laboratory involving fluorescence methods and nucleic acid conformational equilibria to detect nucleic acid/protein interactions. Our project includes application of this methodology in drug discovery and environmental detection of pathogens.

Neutron scattering is used in a wide variety of applications in studies of liquids and solids. Elastic scattering measured as a function of angle is diffraction and is analogous to x-ray diffraction. A major difference, however, is that neutrons scatter from nuclei while x-rays are scattered by electrons. X-ray scattering increases with the atomic number. The scattering of neutrons, generally speaking, does not vary greatly with atomic number but does depend on the particular isotope involved. The usual use of neutron diffraction in studies of crystalline solids is for the precise location of hydrogen atoms. We have recently begun such studies using neutron powder diffraction studies of polycrystalline samples to obtain precise atomic coordinates for samples at 15 K. These studies are performed at the Argonne National Laboratory near Chicago (<http://www.pns.anl.gov>). We are also performing x-ray powder diffraction studies at low temperature at the National Synchrotron Light Source at Brookhaven National Laboratory

Inelastic neutron scattering (INS) spectroscopy is a technique of vibrational spectroscopy that differs from IR and Raman spectroscopy in several respects. One of these is that there are no selection rules in INS so that many vibrations that are not seen by the optical methods can be observed. The most important and unique feature of INS is that the intensity of vibrational transitions is dominated by motions of the hydrogen atoms in the material. If hydrogen is present it dominates the scattering. For example, methyl rotations, which are very weak in other kinds of spectra, are very strong in INS. All other atoms, including deuterium, do not scatter appreciably by comparison. This permits selective deuteration experiments in which parts of a sample are "removed" by substitution of D for H

Most of our inelastic neutron scattering experiments are performed at the NIST Center for Neutron Research (www.ncnr.nist.gov) or at the ISIS facility of the Rutherford Appleton Laboratory (www.isis.rl.ac.uk) south of Oxford in England. At NCNR we use the spectrometer called FANS while at ISIS we use the spectrometer called TOSCA (www.isis.rl.ac.uk/molecularspectroscopy/tosca/). A collection of INS spectra is available at the TOSCA site.

The icosahedral hydrocarbon dodecahedrane, C₂₀H₂₀, is an example of one of our ongoing studies. In a previous study we compared the spectrum computed for this molecule on the basis of an isolated molecule model with the spectrum obtained for the polycrystalline solid. In current work the calculations have been extended to the full periodic solid. The degree of agreement between theory and experiment is now excellent. We are now repeating the determination of the crystal structure of this material using synchrotron radiation and low temperature. It appears that inclusion of the phonon motions in the treatment of the x-ray data is needed in order to obtain a correct C-C bond length for this material.

Divisional Seminars**ORGANIC (940)**

Monday September 5, 2005
2:00p.m.-3:00p.m. - 548 Hah
NO SEMINAR

PHYSICAL (970)

Monday, September 5, 2005
4:00pm - 5:00pm - 548 Hah
NO SEMINAR

BIOCHEMISTRY (930)

Tuesday, September 6, 2005
12:30pm - 1:30pm - 548 Hah
NO SEMINAR

ANALYTICAL (920)

Wednesday, September 7, 2005
2:30pm - 3:30pm - 548 Hah
"Preparing & Giving a Scientific Presentation"

INORGANIC (940)

Thursday, September 8, 2005
3:30pm - 4:30pm - 548 Hah
NO SEMINAR

2005 ACS OFFICERS

Presidents: Nazita Obaidi and Sara Duhachek
Vice Presidents: Chris McCune and Fred Zinnel
Secretary: Jasmine Lee
Treasurer: Curtis Wray
Publications: Molly Ball
ACS Email: acs_unl@hotmail.com

From the Editor's Desk

Articles and/or ideas for this publication can be submitted to Leann Galusha, room 551 Hamilton Hall, Lincoln, NE 68588-0304, (402) 472-3634 or email at lga-lusha2@unl.edu

NEW CHEMISTRY DEPARTMENT STAFF

Leanna Klempa

Leanna Klempa joined the Chemistry Department in July. She is a Staff Secretary III working in the main business office, room 552, in the mornings. She is the receptionist, schedules conference rooms, serves as backup to Mellanie Gilroy with payroll, and assists with various departmental projects, such as the upcoming "Chemistry Day".



Deanna Larson

Deanna Larson joined the Chemistry Department in July. She is the Recruiting and Graduate Admissions Secretary and is located in room 516. She works with the graduate students, the Graduate Recruiting Chair, and Graduate Committee in our department. Deanna works closely with personnel from Graduate Studies and International Affairs.

Leanna and Deanna have been a valuable addition to our Chemistry Department Staff. Please stop by their offices and tap into their resources when you need assistance.

UNL EMPLOYEE SERVICE AWARDS**Friday, September 9, 2005****Service Award Recognition Program**

9:00am - doors open

10:00am - program begins

11:00am - State of the University Address
by Chancellor Harvey Pearlman

Followed by the "All-University Picnic"

Chemistry Department Honorees:**Walt Hancock - 30 years****Jonathan Skean - 25 years****Mike Cook - 20 years****Mark Griep - 15 years****Hadrian Duke - 5 years****Robert Wilson - 5 years****Physics and Astronomy Honorees:****Les Marquart - 35 years****Pat Pribil - 10 years****Hamilton Hall - Renovation News**

Renovation continues on the north wing of 7th and 8th floors until late in the fall. 5th floor and 6th floor halls are in the final stages (including ceiling tiles).

For any questions, concerns or emergencies concerning the renovation please use the following telephone numbers:

*Chair's Office: 472-3634**Mike Cook 472-2685 (Office)**437-1577 (Pager)**Jim Townsley - Shanahan (402) 610-*

UNL Announcements

Fall 2005 Tuition and Fees Due Date

The due date for Fall 2005 tuition and fees will be the second Wednesday of September (Sept. 14th), and not in October as in previous years. Visit the URL below for additional billing information. <http://stuacct.unl.edu/>

EHS COLLOQUIUM SERIES FOR RESEARCH PIs

presents

Personal Protective Equipment (Laboratory) **Dr. Jim Zeigler, DuPont Personal Protection**

Tuesday, September 20, 2005

SEMINAR

Sponsored By: Center for Materials Research & Analysis / NSF-MRSEC

Title: Q & A on Synthesis of Nanoparticles and Nanotubes

Speaker: *Professor Stephen O'Brien*,
Dept. of Materials Science & Engineering,
Columbia University

Date/Location/Time:

Friday, September 16, 2005
217 Ferguson Hall
1:30 p.m.

Morning Session (located in Beadle Center Conference Room N172)

8:30 – 9:30 a.m. Presentation

9:30 – 11:00 a.m. PPE available for viewing, handling, and questions

Afternoon Session (located in Hamilton Hall, Room 110)

2:00 – 3:30 p.m. PPE available for viewing, handling, and questions

3:30 – 4:30 p.m. Presentation

Light refreshments will be available.

*Faculty, Graduate Students and
Laboratory Personnel are encouraged to attend.*

For more information, contact Elizabeth (Betsy) Howe (472-5488 or ehowe2@unl.edu) at EHS. Colloquium Series facilitated by: Environmental Health and Safety (EHS), in cooperation with Grainger, Inc. and DuPont Personal Protection

Nebraska MRSEC 3rd Annual Review & Symposium—SEPT. 20-21

The Third Annual NSF Materials Research Science and Engineering Center Review and Symposium will be held at UNL on Sept. 20 and 21. The Review on Sept. 20 will provide a summary of the new work at Nebraska on “Quantum and Spin Phenomena in Nanomagnetic Structures (QSPINS).” The Symposium on Sept. 21 entitled “Emerging Challenges in Nanomagnetism” will consist of invited talks by the following leading national experts: Sam Bader, Argonne National Lab; Andreas Berger, Hitachi Global Storage Technologies; Eugene Chudnovsky, CUNY; Chris Leighton, University of Minnesota; Sara Majetich, Carnegie Mellon University; David Pappas, NIST; Andrei Slavin, Oakland University. There will be ample opportunity for discussions of future directions of the field. All interested faculty, postdocs and students are invited to attend and are encouraged to present a poster at the Poster/Wine and Cheese Reception at 4:48 p.m. on Sept. 20. Advance registration is required. For additional information and registration information, see our website (www.mrsec.unl.edu) or call Administrative Coordinator Shelli Krupicka (472-7886).