

THE

TarHelium



A Publication of the North Carolina Section of the American Chemical Society

Vol. 21 No. 1

September - October 1990

COMPUTATIONAL CHEMISTRY SYMPOSIUM AND TUTORIAL

Tutorial

September 13, 1990

8:00 pm

Symposium

September 14, 1990

8:30 am - 5:00 pm

September 15, 1990

8:30 am - 12:30 pm

Location

IBM, North Park Bldg.

4800 Falls of the Neuse Road

Raleigh, North Carolina 27609

ACS and Non-ACS Members are invited.

Support for this symposium has been made possible
by generous contributions from:

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NOTES FROM THE EDITOR

Deadlines for the *TarHelium*

October 1, 1990
January 15, 1991
March 15, 1991

Staff Notes . . .

Our search for a new advertising manager ended happily with the signing on of Dr. Linda M. Stroud. Her strong organizational skills (teaching) are an appreciated addition to our *TarHelium* crew. Dr. Bill Switzer continues to put out the meeting notices and I try to handle the four issues of the *TarHelium*. But, as usual, I need your help. We all know someone, somewhere, who really would love!!! to advertise to 1600 interesting chemists. Take this issue of the *TarHelium* to the person in charge of that sort of thing and sell them on what a great bargain we are...

| | |
|-----------|--------------------|
| Full page | \$200/single issue |
| 1/2 page | \$100/single issue |
| 1/4 page | \$50/single issue |

Of course, we have "volume discounts." It is important that your company, service, etc. reach our members and it is important that we have the community and local support. See what you guys can do and send questions as well as business to Dr. Linda Stroud. Thanks and let's make this a great year for our local section. Come to n+1 meetings this year compared to last year...See you at the Computational Chemistry Symposium!

ACS MEETING PROGRAM

Professor Jeffrey Zink
Department of Chemistry
University of California at Los Angeles

Squeezing Light Out of Crystals: Triboluminescence

Monday, October 15, 1990

7:30 pm

Location

Holiday Inn
1301 N. Fordham Street
(highway 15/501 across from Eastgate Mall)
Chapel Hill

Social Hour: 5:30 pm

***Dinner: 6:30 pm**

Lecture: 7:30 pm

Reservations: A reservation is a commitment; please cancel within 4 hours of the meeting to avoid being billed. The cost of the dinner is \$15 for members and guests and \$7.50 for students. Reservations deadline is 4:30 pm, Thursday, October 11, 1990. In Chapel Hill, call Becky Smith - 962-2172; in Durham, call Carolyn Bean - 684-2114; in Raleigh, call Joyce Dunn, 737-545; and in Fayetteville, call Sandra Smith, 486-1669.

Squeezing Light Out of Crystals: Triboluminescence

Dr. Jeffrey I. Zink

Department of Chemistry
University of California at Los Angeles

Triboluminescence (TL) is the light emitted when mechanical energy is applied to a crystal. Many common substances (including sugar and copper sulfate) are triboluminescent. A "hands on" demonstration of the phenomenon will be provided. Five aspects of the TL of molecular crystals excited by the application of mechanical stress will be discussed. First, TL spectroscopy will be described and the excited state origins of the luminescence will be described. Secondly, the mechanical aspects of TL will be described and quantified. The TL is intimately related to the dynamics of crystal fracture. Third, the internal pressures existent during TL will be discussed. Fourth, a general crystal structure requirement will be delineated. Finally, the excitation mechanism based on the above observations will be described.

Biography

Professor Jeffrey Zink is presently Professor of Chemistry at UCLA. He received his B.S. degree from the University of Wisconsin in 1966 and his Ph.D. from the University of Illinois in 1970.

In 1975, he was a Camille and Henry Dreyfus Teacher Scholar; in 1979, the Alexander Von Humboldt Stipendiat; in 1983, the Glenn Seaborg Award Recipient; and in 1987-88, the John Simon Guggenheim Foundation Fellow.

He is a member of the ACS, Interamerica Photochemical Society, National Audubon Society, Phi Kappa Phi and Phi Lambda Epsilon.

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WHAT'S A CHP AND WHY SHOULD I BE CONCERNED?

A final rule on "Occupational Exposures to Hazardous Chemicals in Laboratories" was published by OSHA on January 31, 1990 (Federal Register, p. 3300). Under this new rule known as the laboratory standard, a chemical hygiene plan (CHP) must be in place in most teaching and research laboratories that use or store chemicals by January 31, 1991. This CHP is a written program prepared and implemented by the employer that sets forth procedures, equipment, personal protective equipment, and work practices that will maximize protection of persons working with hazardous chemicals in that area.

If there is sufficient interest, the local section will sponsor a workshop on the laboratory standard and the preparation of a Chemical Hygiene Plan this fall. Please call George Wahl (NCSU) at 737-2941 for further information.

**PROGRAM FOR
CHALLENGES IN COMPUTATIONAL CHEMISTRY**

**4TH ANNUAL SYMPOSIUM OF THE NORTH CAROLINA SECTION
OF THE AMERICAN CHEMICAL SOCIETY**

September 14-15, 1990
McKimmon Center, North Carolina State University

[1] Friday, September 14

8:35 am - 8:40 am **OPENING REMARKS**

A. ELECTRONIC STRUCTURE (Prof. L.G. Pedersen, presiding)

8:40 am - 9:20 am Computation chemistry
for science and technology **Dr. B. Liu**
(IBM-Almaden)

9:20 am - 10:00 am Recent computational advances
in density functional theory **Prof. W. Yang**
(Duke University)

10:00 am - 10:20 am Coffee break

10:20 am - 11:00 am Numerical simulation of molecular
systems in the chemical industry **Dr. D.A. Dixon**
(du Pont)

11:00 am - 11:40 am Bonding and reactivity in organic
and inorganic molecules **Prof. E.R. Davidson**
(Indiana University)

11:40 am - 12:25 pm Panel discussion on electronic
structure **Prof. R.G. Parr**
(UNC-Chapel Hill)

12:25 - 1:30 pm Lunch break

B. CHEMICAL REACTIVITY (Prof. M.H. Whangbo, presiding)

1:30 pm - 2:10 pm Interfacing electronic structure
theory and dynamics **Prof. M.S. Gordon**
(North Dakota State
University)

2:10 pm - 2:50 pm Reaction path **Prof. H.B. Schl**
(Wayne State
University)

| | | |
|-------------------|--|--|
| 2:50 pm - 3:10 pm | Coffee break | |
| 3:10 pm - 3:50 pm | Modelling regio- and stereo-selectivity in organic reactions | Prof. W.J. Hehre (UC-Irvine) |
| 3:50 pm - 4:30 pm | Mechanisms of pericyclic reactions: the biradical problems | Prof. M.J.S. Dewar (UT-Austin) |
| 4:30 pm - 5:15 pm | Panel discussion on chemical reactivity | Prof. W.L. Jorgensen (Yale University) |

C. POSTER SESSION

7:30 pm - 11:00 pm ~ 30 papers

[2] **Saturday, September 15**

D. MODELLING (Dr. S. Profeta, presiding)

| | | |
|---------------------|--|--|
| 8:40 am - 9:20 am | Inside on molecular recognition from solution modelling | Prof. W.L. Jorgensen (Yale University) |
| 9:20 am - 10:00 am | Computer simulation of chemical processes in solution and proteins | Prof. A. Warshel (University of Southern California) |
| 10:00 am - 10:20 am | Coffee break | |
| 10:20 am - 11:00 am | Computer simulation of DNA bending and twisting | Prof. W. Olsen (Rutgers University) |
| 11:00 am - 11:40 am | A new family of antibacterial agents designed from a model of penicillin | Prof. S. Wolfe (Simon Fraser University) |
| 11:40 am - 12:25 pm | Panel discussion on modelling | Dr. E. Wimmer (Cray Research) |
| 12:25 pm - 12:30 pm | CLOSING REMARKS | |

FALL PROGRAM

September 14-15 **Symposium**
Challenges in Computational Chemistry
McKimmon Center
North Carolina State University
Raleigh, NC 2769

October 15 **Dr. Jeffrey Zink**
Squeezing Light Out of Crystals:
Triboluminescence
Holiday Inn, Chapel Hill
Social hour - 5:30 pm
Dinner - 6:30 pm
Lecture - 7:30 pm

November 14 **Dr. Roland Lehr**
Mechanisms of Chemical Carcinogenesis
Duke University, Durham
Faculty Commons
Social hour - 5:30 pm
Dinner - 6:30 pm
Lecture - 7:30 pm
Paul M. Gross Laboratory

December 11 **NC Distinguished Speaker**
Dr. Richard Wolfenden
UNC-CH Dept. of Biochemistry and
Nutrition
Transition State Stabilization by Enzymes
and the Limits of Protein Ligand Binding
Discrimination in Water
Faculty Club, NCSU
Social hour - 5:30 pm
Dinner - 6:30 pm
Lecture - 7:30 pm

CALL FOR PAPERS

The polymer division of the ACS is presenting a Polymer Technology Conference to celebrate its 40th birthday, June 3-5, 1991 at the Wyndham Franklin Plaza Hotel in Philadelphia, PA.

The topics to be feature are:

Barrier Polymers and Constructions

**Enhancement of Polymer Properties Through
Mechanical Or Chemical Means**

High Performance Materials

Applications of Polymers for Biological Systems

Polymers for Designed Applications

Polymers for Hostile Environments

Recyclable Polymers

Solvent-free Chemistry and Technology

For further information, please contact the conference chairman, J.C. Salomone, Rochal Industries, 499 E. Palmetto Park Road, Boca Raton, FL 3343 (407) 451-9260, (407) 395-4100, FAX (407) 451-9269.

CALL FOR NOMINATIONS

for the

GUSTAVUS JOHN ESSELEN AWARD

for

CHEMISTRY IN THE PUBLIC INTEREST

Established in 1985 by the NE section of the ACS, this award annually recognizes a chemist whose scientific and technical work has contributed to the public well-being and has thereby communicated positive values of the chemical profession.

The person who nominates a candidate is requested to provide seven copies of

1. a biography of the candidate
2. a description of their public contribution and its importance
3. copies of pertinent news articles and technical papers
4. the names of three co-sponsors.

Please send nominations and inquiries for further information to:
Chair, Esselen Award Committee, c/o Northeastern Section, American Chemical Society, 19 Mill Road, Harvard, MA 01451, Tel. (508) 456-8227.

Nominations should be postmarked
no later than **December 1.**

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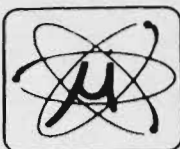
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| ● Failure Analysis | |

For Further Information,
Contact James Ficca (302) 998-1184

Environmental Chemistry - A New Decade of Growth

Eleventh Annual Meeting
Analytical Laboratory Managers Association
Holiday Inn, Research Triangle Park, NC
October 25-26, 1990

For further information, write:
Analytical Laboratory Managers Association
P.O. Box 258
Montchanin, DE 19710
Attention: R.F. Stalzer

The TarHeliium is a publication of the North Carolina Section of the American Chemical Society. The views expressed herein are not necessarily those of the Section.

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