

# Computers in Chemical Education Newsletter Spring 1997

Molecular Orbital Theory

HyperChem - oxygen.hin

File Edit Build Select Display Databases  
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Oxygen

Oxygen

This is the MO theory energy level diagram for the oxygen molecule. Click on each energy level to see the corresponding molecular orbital

Energy

Question 1 Question 2 Question 3

← → Menu Index Exit

Alpha: Orbital Index = 5 Orbital Energy = -17.304726[eV]

Editor Brian Pankuch, Department of Chemistry, Union County College, Cranford, NJ 07016  
pankuch@hawk.ucc.edu.

**Submissions:** General articles should be sent to editor Brian Pankuch at the above address. We would appreciate both 1) printed copy (hardcopy) and 2) a readable file on a Macintosh or IBM compatible 3 1/2" diskette. We have fewer problems with 3 1/2" diskettes. Email submissions are frequently lost, and formatting and special characters are changed.

**Submission deadlines:** Fall issue - Sept. 25; Spring issue - March 15.

Email submissions are frequently lost, and formatting and special characters are lost.

**ALL NEW AND RENEWAL SUBSCRIPTIONS: PLEASE SEND REMITTANCE TO:**

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**RATES:** USA 1 year \$2.50, two years \$4.50; Other countries 1 yr \$5, two yr \$9. Please make a check or money order payable in US funds to Computers in Chemical Education Newsletter. Two issues are published per year.

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Cover: A ToolBook Front-End for a Molecular Modeling Program      David Whisnant

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Studio, Director and SoundEdit 16 from Macromedia. ( 1-800-288-4797).  
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## 24...FROM THE CHAIR

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## FROM THE CHAIR

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## SUMMER 1997 ON-LINE CONFERENCE June 1 to August 1, 1997

Eleven papers will be presented at the Summer 1997 On-Line Conference featuring "General Papers in Chemistry and Chemical Education". The papers and their authors are:

### Paper 1: USING NETSCAPE AS A PRESENTATION MANAGER

Scott E. Van Bramer, Widener University, Chester, PA 19013. svanbram@science.widener.edu, <http://science.widener.edu>

### Paper 2: ASSESSMENT IN CHEMISTRY/NEW STRATEGIES FOR NEW TIMES

I. Dwaine Eubanks, ACS DivCHED Examinations Institute, Clemson University, Clemson SC 29634 eubanki@clemson.edu

### Paper 3: WHAT EVERY CHEMIST SHOULD KNOW ABOUT COMPUTERS, II

Mary L. Swift, Department of Biochemistry and Molecular Biology, College Of Medicine, Howard University, Washington DC 20059-0001. mswift@umd5.umd.edu, and  
Theresa Julia Zielinski, Chemistry Department, Niagara University, Niagara University, NY 14109. theresaz@localnet.com

### Paper 4: THE COSTS OF INCORPORATING INFORMATION TECHNOLOGY IN EDUCATION

Brian M. Tissue, Department of Chemistry, Virginia Polytechnic Institute and State University, Blacksburg, VA 24061-0212. tissue@vt.edu

### Paper 5: USING PSEUDOSCIENCE TO TEACH GENERAL AND ANALYTICAL CHEMISTRY

Michael Epstein, Margaret Bullard, Brad Buehler, Robin Koster, Department of Science, Mount Saint Mary's College, Emmitsburg, MD 21727. epstein@msmary.edu

### Paper 6: NATURE DOESN'T SOLVE EQUATIONS, SO WHY SHOULD WE? MATHEMATICALLY-LEAN SIMULATIONS IN CHEMISTRY

Hugh M. Cartwright, Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, England OX1 3QZ. hugh@muriel.pcl.ox.ac.uk

### Paper 7: SUPPLEMENTAL INSTRUCTION: A MODEL PROGRAM THAT GOES AGAINST THE GRAIN

Cory Emal, Tanya Johnson and Paul Kelter, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304. pkelter@unlinfo.unl.edu

### Paper 8: THE USE OF EXCEL IN PHYSICAL CHEMISTRY SEMINARS

A. A. Kubasov, V. S. Lyutsarev and K. V. Ermakov, Moscow State University, Russia. kubasov@comp.chem.msu.su

### Paper 9: ARE SIMULATIONS JUST A SUBSTITUTE FOR REALITY?

Harry E. Pence, Chemistry Department, SUNY Oneonta, Oneonta, NY, 13820. pencehe@oneonta.edu

### Paper 10: ENVIRONMENTAL AND INDUSTRIAL CHEMISTRY: AN ON-LINE INTERCOLLEGIATE COURSE

Leonard J. Archer (1), James M. Beard (2), Sylvia R. Esjornson (3), Aline M. Harrison (4), Reed Howald (5), Peter Mahaffy (6), Maria Pacheco (7), Donald Rosenthal (8), Mary M. Schreiner (9), and James N. Stevenson (10). rosen1@clvm.clarkson.edu

- (1) Missouri Western State College, St. Joseph, MO
- (2) Catawba College, Salisbury, NC
- (3) Southwestern Oklahoma State University, Weatherford, OK
- (4) York College of Pennsylvania, York, PA
- (5) Montana State University, Bozeman, MT
- (6) The King's University College, Edmonton, Alberta, Canada
- (7) SUNY- Buffalo State College, Buffalo, NY
- (8) Clarkson University, Potsdam, NY
- (9) Niagara University, Niagara University, NY
- (10) Concordia University, Austin, TX

### Paper 11: CHEMISTRY ON-LINE: A PRACTICAL GUIDE TO THE DEVELOPMENT OF INTERACTIVE, INTERCOLLEGIATE LEARNING EXPERIENCES FOR CHEMISTRY STUDENTS

George R. Long, Department of Chemistry, Indiana University of Pennsylvania, Indiana, PA 15705

REGISTRATION AND PARTICIPATION

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SCHEDULE

June 1 to June 20 - On-Line Session 1

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- On or before June 1 - Retrieve Papers 1 to 5
- June 2 - Short Questions for Paper 1
- June 3 - Short Questions for Paper 2
- June 4 - Short Questions for Paper 3
- June 5 - Short Questions for Paper 4
- June 6 - Short Questions for Paper 5

- June 9 and 10 - Discussion of Paper 1
- June 11 and 12 - Discussion of Paper 2
- June 13 and 16 - Discussion of Paper 3
- June 17 and 18 - Discussion of Paper 4
- June 19 and 20 - Discussion of Paper 5

June 23 to July 11- On-Line Session 2

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- On or before June 22 - Retrieve Papers 6 to 8
- June 23 - Short Questions for Paper 6
- June 24 - Short Questions for Paper 7
- June 25 - Short Questions for Paper 8

- June 30 and July 1 - Discussion of Paper 6
- July 7 and July 8 - Discussion of Paper 7
- July 9 and July 10 - Discussion of Paper 8

July 14 to Aug. 1 - On-Line Session 3

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- On or before July 13 - Retrieve papers 9 to 11
- July 14 - Short Questions for Paper 9
- July 15 - Short Questions for Paper 10
- July 16 - Short Questions for Paper 11

- July 21 and 22 - Discussion of Paper 9
- July 23 and 24 - Discussion of Paper 10
- July 25 and 28 - Discussion of Paper 11

July 29 to August 1 - General Discussion and Evaluation

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ABSTRACTS OF PAPERS

Abstracts for the eleven conference papers are available on the CHEMCONF World Wide Web Site.

(The URL is <http://www.wam.umd.edu/~toh/ChemConf97.html>)

Anyone may register for and participate in this on-line conference. There is no registration fee. To register for CHEMCONF send the message: SUBSCRIBE CHEMCONF your-first-and-last-name To: LISTSERV@UMDD.UMD.EDU Conference information and announcements will be distributed via CHEMCONF.

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1997-1998 SCHOOL YEAR ON-LINE SESSIONS

In addition to the summer sessions, there will be school year sessions. The format of the school year sessions is that one week will be devoted to the discussion of each paper. Short questions will be sent on Friday and discussion will occur on Monday through Thursday. The fall semester session will occur between September 5 and November 26, 1997. The spring semester session will occur between January 30 and May 1, 1998. A number of papers have already been promised. Additional authors should contact Thomas O'Haver (to2@umail.umd.edu, 301-405-1831). The deadlines for school year papers are:

- June 1, 1997 - Deadline for title and abstract
- July 1, 1997 - School year session schedule will be established and distributed
- August 1, 1997 - Deadline for receipt of papers for September to December session.
- January 1, 1998 - Deadline for receipt of papers for February to May session.

## FROM THE CHAIR

**Donald Rosenthal, Chair CCCE (Committee on Computers in Chemical Education)**  
Department of Chemistry Clarkson University  
Potsdam NY 13699-5810  
Phone: 315-268-2352  
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### A. ROLE OF THE COMMITTEE

The CCCE seeks to publicize and promote the use of computers in chemical education.

### B. MEMBERS OF THE COMMITTEE - 1997

Charles Abrams - McGill University, Montreal, Canada  
James Beard - Catawba College, Salisbury, N  
James W. Beatty - Ripon College, Ripon, WI  
Joseph Casanova - California State University, Los Angeles, CA  
Wilmon B. Chipman - Bridgewater State College, Bridgewater, MA  
Nancy S. Gettys - University of Wisconsin, Madison, WI  
William Halpern - University of Western Florida, Pensacola, FL  
Carolyn Sweeney Judd - Houston Community College, Houston, TX  
Alfred Lata - University of Kansas, Lawrence, KS  
Yuzhuo Li - Clarkson University, Potsdam, NY  
George R. Long - Indiana University of Pennsylvania, Indiana, PA  
Marco Molinaro - University of California, Berkeley, CA  
Thomas C. O'Haver - University of Maryland, College Park, MD  
Brian Pankuch - Union County College, Cranford, NJ  
Harry E. Pence - SUNY College, Oneonta, NY  
Donald Rosenthal - Clarkson University, Potsdam, NY  
Gwen Sibert - Roanoke Valley Governor's School, Roanoke, VA  
Stanley Smith - University of Illinois, Urbana, IL  
Carl H. Snyder - University of Miami, Coral Gables, FL  
Brian Tissue - VPI and State University, Blacksburg, VA  
David M. Whisnant - Wofford College, Spartanburg, SC  
Theresa J. Zielinski - Niagara University, Niagara University, NY

### C. ON-LINE MEETINGS AND SYMPOSIA

An on-line Conference entitled "General Papers in Chemistry and Chemical Education" will be held during the summer of 1997 and the 1997-1998 school year. See the article elsewhere in this Newsletter for additional details.

Anyone interested in organizing a three to five week (5 paper) session at a future (1998 and beyond) on-line meeting should contact me (ROSEN@CLVM.CLARKSON.EDU). I would also like to hear from anyone interested in managing a meeting Listserv or Website.

### D. ON-LINE INTERCOLLEGIATE COURSES

The CCCE sponsored and helped organize an intercollegiate course entitled "Environmental and Industrial Chemistry". This course will be described and discussed in this year's summer on-line conference (Paper 10). In addition, George Long will present a paper (Paper 11) entitled "Chemistry On-Line: A Practical Guide To The Development Of Interactive, Intercollegiate Learning Experiences For Chemistry Students".

I would be interested in hearing from those who are willing to help organize an on-line course.

### E. NATIONAL COMPUTER WORKSHOPS

Three day National Computer Workshops were held last summer before the BCCE at Clemson University. There were a total of 68 registrants for these workshops. It seems likely that similar Workshops will be held before the 1998 BCCE at the University of Waterloo. More information about these Workshops will be included in the Fall 1997 issue of this Newsletter.

### F. CCE NEWSLETTER

The publication of this Newsletter represents a major activity of the Committee on Computers in Chemical Education. Articles submitted for publication are printed in a timely manner. Anyone interested in submitting an article should contact Brian Pankuch, Editor of the CCE Newsletter (PANKUCH@HAWK.UCC.EDU) or me.

### G. OPEN MEETING AT BCCE MEETINGS

In recent years, the CCCE has held open meetings at the Biennial Meetings. These are well attended and provide an opportunity for interaction between Committee members and those attending. A meeting was held at Clemson and another meeting is planned for the 1998 BCCE at the University of Waterloo.

### H. WE ALWAYS NEED IDEAS AND SUGGESTIONS

The success of the Committee depends upon our interaction with you and other chemical educators. Please send us your ideas and suggestions.