The Lattice

MSA and the Geochemical Society offer short course on molecular modeling theory by Randall T. Cygan

heMineralogical Society of America and the Geochemical Society are combining efforts in offering the opportunity for students and professionals to learn about the role of molecular modeling in mineralogical and geochemical systems. A short course entitled "Molecular Modeling Theory and Applications in the Geosciences" will be held in Roanoke, Virginia on May 19-20, 2001. The organizers of the course are Randall Cygan of Sandia National Laboratories and James Kubicki of Pennsylvania State University. The short course, which will precede the 2001 Goldschmidt Conference in Hot Springs, Virginia, will cover some of the most important and timely information on atomistic and molecular simulations of mineral systems.

Molecular modeling methods have become important tools in many areas of geochemical and mineralogical research. The purpose of this course will be to help introduce molecu-

lar modeling to researchers considering moving into this expanding field and to familiarize experimentalists with the type of information available from computer simulations. The short course will focus on techniques and applications for modeling a wide variety of problems in mineralogy and geochemistry. Techniques covered will include energy minimization, lattice dynamics, Monte Carlo methods, and molecular dynamics. Important concepts of quantum mechanics and electronic structure calculations, including both molecular orbital and density functional theories, will be introduced. Applications will cover a broad range of mineralogy and geochemistry topics-from atmospheric reactions to properties of mantle and core phases. Throughout the course, emphasis will be placed on the comparison of molecular simulations with experimental data and the synergy that can be generated by using both approaches in tandem. Those interested in using molecular modeling in research or understanding papers in computational chemistry should attend. This short course will provide a lively forum for discussions of theory, simulations, computers, spectroscopy, experiments, and their link with field observations.

For additional information and registration materials for this short course, **see pages 8–9 of this issue** of *The Lattice*, or visit the short course web page at www.sandia.gov/eesector/GScourse.htm.

2001 Nominees for MSA Office

The following is the slate of officer nominees for the Council year 2002:

Vice Presidential nominees:

Stephen J. Guggenheim (University of Illinois-Chicago) Douglas Rumble (Carnegie Institution, Geophysical Lab)

Secretary:

David M. Jenkins (State University of New York-Binghamton)

Councillors: (in alphabetical order) James M. Brenan (University of Toronto) Peter J. Heaney (Pennsylvania State University) Nancy L. Ross (Virginia Polytechnic Institute) Bernard J. Wood (University of Bristol)

The Newsletter of the Mineralogical Society of America

Subscription and membership information is on page three.

1015 18th Street, N.W., Suite 601, Washington, D.C. 20036-5212 U.S.A. ISBN 1526-3746

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Changes in The Lattice; thoughts on undergraduate mineralogy

by Cornelis ("Kase") Klein, MSA President

Recipients of the November 2000 issue of The Lattice, which arrived probably sometime in early February 2001, will have noticed that it has a quite different look from earlier issues. This is the result of two factors: a change-over in editors, as well as the decision to do the complete lay-out of the newsletter in the editorial offices of MSA in Washington, D.C. Let me express our collective gratitude, on behalf of MSA, to the editor of The Lattice for the past five years, Darrell Henry of Louisiana State University, Baton Rouge. He has given very generously of his time to provide MSA with a most informative newsletter. Many thanks, Darrell. Let me also remind you

that another member of the Geology Department at Louisiana State has also shown great commitment to the Society, namely Barb Dutrow. She was the Secretary of the Society for four years, between 1996 and 1999. These two members of the same department have done yeoman service for the Society. Many, many thanks to both of you!

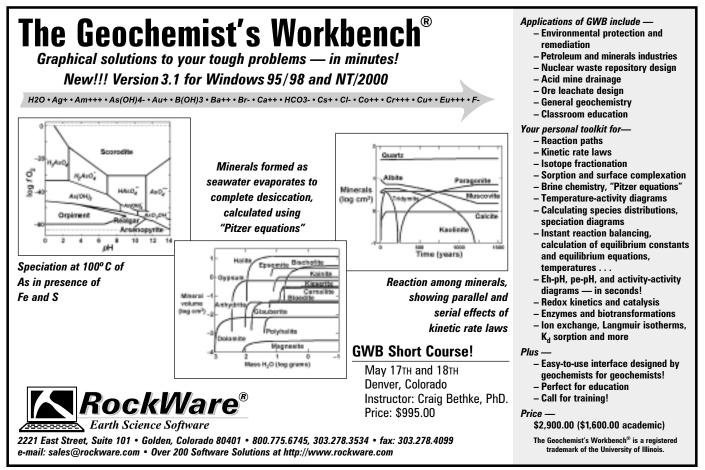
Our new editor, beginning with this February issue, is Andrea Koziol of the University of Dayton, Ohio. We look forward to many more years of successful issues under her editorship.

Let me now bring up an issue that, I think, has been of serious concern for many years with a considerable segment of the membership of MSA. I will

introduce it as "Some thoughts about the teaching of the undergraduate mineralogy course in North American Universities." Others have addressed this issue in earlier years. A good example is the Comments column, written by John Brady of Smith College in 1995 in Geotimes (Sept. issue, p. 5) entitled "Confessions of a Mineralogy Professor." He begins with a statement of a well-known secret: Minerals are the most interesting objects on Earth, and they are fun to study. He continues by asking the question "why then do geologists feel such a lack of enthusiasm for mineralogy?" His quick answer is "Because most geologists once took a course in mineralogy-and it was not very

good." This is a serious issue and the quality of the undergraduate mineralogy course very much affects the student's enthusiasm (or the lack thereof) for mineralogy, which in turn has a strong influence on the future path that is selected in further professional training. In the long run it affects what students will do in graduate school and even, whether or not they will join a society such as ours, the Mineralogical Society of America. Here follow some of my thoughts on the subject.

Over the last twenty years or so, Geology (or Earth Science, or Earth and Planetary Science, and so on) undergraduate curricula have undergone major Continued on page 16





Notes from Washington

by J. Alexander Speer, MSA Executive Director

• Renewal Notices for 2001 were sent to members and subscribers in November 2000. If you did not receive yours, please contact the Business Office. If you did, and have not yet returned it, please renew as soon as possible to save your Society the expense of a second renewal notice. You can renew online if you pay by credit card, or by returning the paper renewal notice with payment. When you renew, please check to make sure your e-mail address printed on your renewal form is correct. You can also check to see what e-mail address we have for you in the online MSA membership Directory and, if incorrect, you can send us an update online. MSA would like to take better advantage of electronic communications with its members but cannot do so if a third or more of its members cannot be reached that way.

• There have been some staff changes in the MSA Editorial Office. Lisa M. Koch, the *American Mineralogist* Production Editor, left us on 9/8/2000 to work in the telecommunication industry. Eric T. Baker, who joined us on 10/16/2000 is now the journal's Production Editor.

• Reviews in Mineralogy and Geochemistry (RiMG) volume 40, *SULFATE MINERALS* - *Crystallography, Geochemistry, and Environmental Significance*, is now available. A general description of the book and the Table of Contents are given on the MSA website at www.minsocam.org. The book accompanies the short course of the same name on November 11-12, 2000. C.N. Alpers, J.L. Jambor and D.K. Nordstrom are the editors of this newest RiMG volume. You can order your copy using the order form elsewhere in this issue, online, or by mail, e-mail, phone, or fax.

"Mineral Structures and Behaviors" Special Session at Goldschmidt 2001

The Mineral Structures Special Interest Group of MSA is sponsoring a special session at Goldschmidt 2001 (May 20-24, 2001) on "Mineral Structures and Behaviors." The keynote speaker is Alain Baronnet, and response to date suggests that this will be a very exciting session. Anyone working in the area of structures and behaviors of minerals and related materials, including: spectroscopy, high pressure/temperature mineralogy, phase transitions, X-ray and neutron diffraction, mineral surfaces, TEM, X-ray spectroscopy, etc. is encouraged to submit an abstract to this session. The deadline for abstracts is Feb. 9th by paper and Feb. 16th for electronic submissions. For additional information see the Goldschmidt website: http:// www.lpi.usra.edu/meetings/gold2001/.

This should be an excellent meeting for those interested in mineral structures; we hope to see you in May. For information on the Mineral Structures session, please feel free to contact the co-organizers: Jeffrey Post (post.jeffrey@nmnh.si.edu) and David Veblen (dveblen@jhu.edu).

The Lattice is published quarterly (February, May, August, November) by the Mineralogical Society of America. It is distributed to MSA members as a service. Articles and letters are welcome.

The Mineralogical Society of America is composed of individuals interested in mineralogy, crystallography, and petrology. Founded in 1919, the Society promotes, through education and research, the understanding and application of mineralogy by industry, universities, government and the public.

Membership benefits include: American Mineralogist, published bi-monthly; 25% discount on volumes in the *Reviews in Mineralogy and Geochemistry* series; *The Lattice*; special subscription rates for *Mineralogical Abstracts, Physics and Chemistry of Minerals, Journal of Petrology*, and *Rocks and Minerals*; reduced registration fees at MSA short courses; member rates for the MSA/ Geological Society of America annual meeting and member rates at MSA's spring meeting with the American Geophysical Union; participation in a Society that supports the many facets of mineralogy.

Dues for 2001: professional members \$50; student members \$5. American Mineralogist subscription: professional members add \$30; student members add \$25. Membership is on a calendar year basis. Individuals who join after January 1, 2001 will be sent all back issues of volume 85 for 2001.

Additional membership information and an application, and/or a price list of the Society's publications are elsewhere in this newsletter, or contact the Business Office.

Institutions may subscribe to the 2001 volume of *American Mineralogist* for the annual rate of \$480 in the US and \$490 for non-US addresses. The subscription price includes any new volumes of the *Reviews in Mineralogy and Geochemistry* series published during the calendar year of the subscription. Payment must be received in full before a subscription will be started.

2001 President: Cornelis Klein, Univ. of New Mexico Past-President: William D. Carlson, Univ. of Texas-Austin Vice President: Rodney C. Ewing, Univ. Michigan Secretary: David Jenkins Binghamton Univ. Treasurer: James G. Blencoe, Oak Ridge Nat. Lab. Editor of The Lattice: Andrea Koziol, Louisiana St. Univ. MSA Executive Director: J. Alexander Speer Production Manager: Rachel A. Russell

Mineralogical Society of America 1015 Eighteenth Street N.W., Suite 601 Washington, D.C. 20036-5212, U.S.A. Tel: (202) 775-4344; Fax: (202) 775-0018 **E-mail:** business@minsocam.org, or Andrea.Koziol@notes.udayton.edu



MSA Award and Office and Nominations

Member participation is essential to the formation and continuation of MSA programs. Involvement can take several forms: nominate a candidate for an award, volunteer to serve on a committee next year, or offer your name or that of a colleague as a possible candidate for office. It is through the involvement of individual members that the Society's programs develop to meet the needs of its members. Please take a minute to read the brief committee descriptions below and consider getting involved. More information about each award and the list of 2001 MSA Committee members are available at the MSA website at www.minsocam.org. Contact the appropriate Committee Chair with your recommendations.

| Award/Office | Deadline | Committee Chair |
|--|----------|--|
| The Roebling Medal is MSA's highest award and is given for eminence as represented by outstanding published original re- search in mineralogy. | June 1 | Michael A. Carpenter Univ of Cambridge Dept Earth Sciences Downing St Cambridge, CB2 3EQ ENGLAND Tel: +44 (1223) 33-3483 Fax: +44 (1223) 33-3450 E-mail: mc43@esc.cam.ac.uk |
| The Dana Medal is intended to recognize continued outstand- ing scientific contributions through original research in the min- eralogical sciences by an individual in the midst of their career. | June 1 | Sorena S. Sorensen Smithsonian Institution Min- eral Sciences NHB119 Washington, DC 20560- 0119 Tel: (202) 357-4010 Fax: E-mail: sorena@volcano.si.edu |
| Mineralogical Society of America Award is give for outstand- ing published contribution(s) prior to 35th birthday or within 7 years of the Ph.D. | June 1 | David L. Bish Geology and Geochemistry Los Alamos National Laboratory, Mail Stop D469 Los Alamos, NM 87545 ph: (505) 667-1165 fax: (505) 665-3285 e-mail: bish@lanl.gov |
| Distinguished Public Service Medal is awarded for distin- guished contributions to public policy and awareness about mineralogical topics. | June 1 | W. Gary Ernst Stanford University Dept Geol & Environ Sci Stanford, CA 94305-2115 Tel: (650) 723-2750 Fax: (650) 725-0969 e-mail: ernst@pangea.stanford.edu |
| Society Fellowship is the recognition of a member's signifi- cant scientific contributions. Nomination is undertaken by one member with two members acting as co-sponsors. Form re- quired, contact committee chair or MSA home page. | June 1 | Robert J. Bodnar Virginia Polytech Inst Dept Geo- logical Sciences Blacksburg, VA 24061-0420 Tel: (540) 231-7455 Fax: (540) 231-3386 e-mail: bubbles@vt.edu |
| MSA Office is open to any non-student member or fellow of the Society. One-year terms for President and Vice-President; two-year terms for treasurer and secretary; three-year term for Councillors. | June 1 | Kathryn Nagy University of Colorado Dept Geo- logical Sci Campus Box 399 Boulder, CO 80309- 0399 Tel: (303) 492-2763 Fax: (303) 492-2606 E-mail: kathryn.nagy@colorado.edu |
| Committee membership is open to any member or fellow of the Society. Terms usually from one to six years. In addition to above committees, there are committees on Management, Meetings, Financial Advisory, Publications, Short Course, Tell- ers, Committee on Committees, Outreach, Arts Council. If you are interested in serving, contact the chair. | April 30 | Rodney C. Ewing Univ of Michigan Dept Nuclear Engineering 2355 Bonisteel Blvd Ann Arbor, MI 48109-2104 ph: (734) 647-8529 fax: (734) 647-8531 e-mail: rodewing@umich.edu |

MSA web site: click it out! WWW.minsocam.org

Announcing the new 22nd Edition of Klein's classic Manual of Mineralogy

now called Manual of Mineral Science!

Manual of Mineral Science, Twenty Second Edition

Cornelis Klein, The University of New Mexico ISBN: 0-471-25177-1, 704 Pages, Cloth. 2002

The new 22nd edition is available this Spring with a wealth of new and revised material.

Cornelis Klein has crafted this edition to remain simply the most effective text of its kind available.

Here are some of new features you'll find in the 22nd Edition:

- * The first seven chapters, now with a different order and packaging of subject matter, can be taught independently and in any sequence.
- * New Introductory Statements provice a preview of the material to be studied.
- * New "Interest Boxes" relate mineralogy to matters that are of more general and/or geologic interest.
- * New fgures and illustrations help with student comprehension of key concepts.
- * Now includes eight new color plates with photographs of 72 of the most common minerals.
- * Each copy includes Mineralogy Tutorials V. 2.1 CD-ROM providing a useful aid to students of all learning styles.

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MINERALOGICAL ASSOCIATION OF CANADA SHORT COURSE

Principles and Applications of Laser Ablation-ICP-Mass Spectrometry in the Earth Sciences

ST. JOHN S, NEWFOUNDLAND

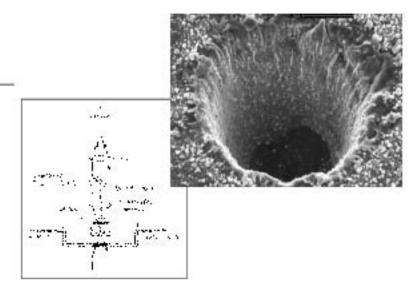
26-27 MAY 2001

(HELD IMMEDIATELY PRECEDING THE JOINT ANNUAL MEETING OF THE GEOLOGICAL ASSOCIATION OF CANADA – MINERALOGICAL ASSOCIATION OF CANADA)

ASER ablation-ICPMS is arguably the most exciting new analytical development in geochemistry in the last decade, opening up approaches to pure and applied geologic problems that were only dreamed of before. The goal of this course is to teach graduate students and post-graduate researchers how laser ablation-ICPMS works, what is being done in the Earth sciences with the method now, and what could be done in the future. It will appeal to all those Earth scientists who are interested in solving geologic problems with chemical data. Material will be presented at the level of understanding of most graduate students in the Earth sciences and will be assembled in a short-course volume.

Technical topics discussed include: Nd-YAG and excimer laser instrumentation; laser beam delivery systems; ablation cell design; quadrupole, magnetic sector and time-of-flight ICPMS instrumentation; collision cell technologies; sample preparation; data acquisition, calibration and quantification strategies; laser ablation phenomena and element fractionation.

Examples of Earth sciences applications: whole rock geochemistry using fusion disk analyses; lithophile element studies of silicate and oxide minerals in the mantle and crust; noble metal element studies of sulphides, oxides and metals in ores and rocks; experimental mineral-melt partitioning; melt inclusions and magmatic processes; fluid inclusions and ore genesis; metamorphic minerals and diffusion-rate processes; trace-element geothermometry/ geobarometry; environmental pollution tracing and monitoring; radiogenic isotope systematics of minerals; U-Pb accessory mineral geochronology.



Registration costs: CAN\$250 for professionals and CAN\$150 for students (includes short-course volume and two cold lunches).

To register and for other information, visit the St. John § 2001 GACMAC website at www.geosurv.gov.nf.ca/stjohns 2001 or contact Dr Paul Sylvester at pauls@sparky2.esd.mun.ca for answers to specific questions.

Online registration will commence on 1 March 2001.

Scheduled Lecturers

Detief Günther, Professur für Analytische Chemie und Spurenanalytik, ETH Zürich, Switzerland

Simon Jackson, Lecturer, School of Earth Sciences, Macquarie University, Australia

Jan Kosler, Lecturer, Department of Geochemistry, Charles University, Czech Republic; and Research Associate, Department of Earth Sciences, Memorial University of Newfoundiand

Henry Longerich, Professor Emeritus, Department of Earth Science, Memorial University of Newfoundland

Nuno Machado, Professeur associ et Agent de recherche et de planification, Sciences de la Terre, Universit du Qu bec à Montr al

Paul Mason, Research Officer, Faculty of Earth Sciences, University of Utrecht, The Netherlands

Marc Norman, Senior Research Fellow, School of Earth Sciences, University of Tasmania, Australia

Paul Sylvester, Associate Professor, Department of Earth Sciences, Memorial University of Newfoundland

Geoff Velnott, Research Scientist, Department of Fisheries and Oceans. Environmental Sciences Division, Northwest Atlantic Fisheries Centre

Student Registration Grants

A limited number of awards is available to students to cover the registration fee. Applicants should send a brief statement outlining their interest in the short course and explaining how their attendance will enhance their academic studies or research to Dr Paul Sylvester by email at **paule@sparky2.esd.mun.ca**. APPLICATIONS MUST BE RECEIVED BY 1 MARCH 2001.



Mineralogical Association of Canada Association minéralogique du Canada P.O. Box 78087, Meriline Postal Outlet 1460 Merivale Road, Ottawa ON Canada, K2E 181 Tel. & fax: (613) 226-4651

All About Color

By Rachel A. Russell, Managing Editor, American Mineralogist

The MSA Council has recently approved a plan to facilitate and encourage the use of color in manuscripts published in the *American Mineralogist*. A special Color Fund has been established, to be used at the Editors' discretion, to support the use of color figures in the manuscripts. Authors are still encouraged to cover a part of the cost, as funds are limited, but the use of color when needed is encouraged.

However, even better news is that the cost of color printing in *American Mineralogist* seems to be considerably less than most Earth Sciences journals. Right now, authors pay only what is clearly indicated on the printer's bill to be the extra costs associated with color. This could include a color separation, the film output, and the actual cost of the color printing. Although the size of the image plays a large factor, the last several bills have been about \$800. The even better news, and little known, is that once color is "open" on a signature of paper, there will be several other pages of color available to that author. Additional figures would be just the cost of separations, perhaps \$100 or so, all depending on size.

And that separation fee can be almost eliminated by submitting a high-quality electronic file. I strongly prefer the tiff files, saved at 300 dpi. If the figure has labels or arrows, the dpi probably should be higher. Right now, the printer can send us a color "proof" of an electronic file for about \$15. Many journals skip this step completely, because if the authors provide the color image file, then presumably it is exactly how they want it. We are still working out how to process electronic color art on a case by case basis, but it seems much easier than hardcopy! I strongly encourage this trend.

The bottom line right now is that if you provide the electronic color file and are flexible about the placement of color in your article, then about \$800 could obtain up to 8 pages to put color figures on. As everyone knows, we send proofs to the authors, so the layout won't be a surprise. In the case of complex color, it could be possible to send another proof, if the layout had to be adjusted because of left/right page alignments. What must be avoided are changes to the color file, whether it is electronic or hardcopy when you submit it. Even the smallest change could be quite expensive! So we try to make sure that the file is good right from the start and get any problems solved before the printer is involved.

Furthermore, if color is necessary to your paper and you have no funds, apply to the Editors for consideration from the Color Fund. I want to encourage authors to add a note to their cover letter, when they initially submit their paper, explaining briefly the importance of the image and how much they could contribute. Right now, if the editors intend for the Color Fund to be used, they let me know when they send me the accepted file. If there is any confusion, I try to clear it up immediately with the authors and editors.

But there is more good news! It turns out that the more

color we use, the cheaper the color is for everyone, due to economies the printer can apply. Occasional pieces of color are expensive, but if it is known that each issue will have, for example, 20 pieces of color or so, then the cheaper it becomes. Much depends on whether few authors use a lot of color (less expensive), or whether many authors use a little (more expensive). MSA could decide to increase the Color Fund, or donations could increase it. Donations can be made to this fund by contacting Alex Speer, MSA's Executive Director, and this would be a tax-deductible type of donation.

We can also consider requests for two colors (versus the 4-color above), and that would be another learning adventure. Another option could be printing a figure in black and white in the journal but providing a color jpeg for the web site. There is a dizzying array of options available right now.

The future of American Mineralogist looks to be quite colorful!

Call for Papers

American Mineralogist honors Holdaway with Special Issue

Barb Dutrow, Special Associate Editor American Mineralogist

s a follow up to the GSA topical session in honor of the retirement of M.J. Holdaway: "Metamorphic petrology from the field to experiments," the *American Mineralogist* has agreed to publish a "Holdaway Issue," to mail March 2002.

We invite contributions for this volume. Any aspect of original research appropriate for publication in the American Mineralogist is welcome. Manuscripts will undergo standard *American Mineralogist* review procedures. Manuscripts can be **submitted from now until about April 30**, but the sooner submitted the more time for revision (if needed). In order for a timely publication, REVISED manuscripts will need to be returned by October 1, 2001.

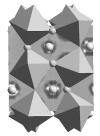
Manuscripts should be sent to: American Mineralogist, 1015 18th St NW Suite 601, Washington, D.C. 20036-5212, USA. Please mention "Holdaway issue" in the cover letter.

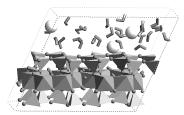
If you have any questions concerning submission, please contact me (dutrow@geol.lsu.edu) or the editorial office. Also, please pass this information along to your co-authors. We look forward to your manuscript!

Read the American Mineralogist. now 8 times a year!

Geochemical Society and Mineralogical Society of America Short Course

Molecular Modeling Theory and Applications in the Geosciences





Not olecular modeling has become an important tool in many areas of geochemical and mineralogical research. The purpose of this course will be to introduce molecular modeling to researchers considering moving into this growing field and to familiarize experimentalists with the type of information available from computer simulations. Although one may never become a full-time molecular modeler, it will be increasingly important to understand these techniques in order to merge experiment and theory. This course will focus on techniques and applications for modeling a wide variety of problems in mineralogy and geochemistry. Techniques covered will include energy minimization (determining structures), lattice dynamics (calculating thermodynamic properties), Monte Carlo (generating configurations in complex systems), and molecular dynamics (predicting dynamic properties such as diffusion rate and viscosity). Important theoretical concepts of quantum mechanical calculations (both molecular orbital and density functional theories) will be introduced. Applications will run the gamut of geochemistry—from atmospheric reactions to properties of mantle and core phases. Throughout the course, emphasis will be placed on the comparison of simulations with experimental data and the synergy that can be generated by using both approaches in tandem. Those interested in using molecular modeling in research or understanding papers in computational chemistry should attend.

Dates: Saturday and Sunday May 19 and 20, 2001 (preceding the Goldschmidt Conference in Hot Springs, Virginia, USA)

Location: Hotel Roanoke and Conference Center in downtown Roanoke, Virginia, USA; 110 Shenandoah Avenue, Roanoke, Virginia 24016, USA; Phone: 540-985-5900; Fax: 540-853-8290

Conveners: *Randall T. Cygan,* Geochemistry Department, Sandia National Laboratories, Albuquerque, New Mexico 87185-0750, USA; Phone: 505-844-7216; E-mail: rtcygan@sandia.gov

James D. Kubicki of Pennsylvania State University, University Park, Pennsylvania 16802, USA, Phone: 814-865-3951; E-mail: kubicki@geosc.psu.edu

Speakers/Authors and Topics:

Randall T. Cygan (Sandia National Laboratories): Molecular modeling in mineralogy and geochemistry **Mihali Felipe** (Yale University): Transition state theory in geochemistry

Julian D. Gale (Imperial College): Simulating the crystal structures and properties of ionic materials from interatomic potentials

Stephen H. Garofalini (Rutgers University): Molecular dynamics simulations of silicate glasses and glass surfaces **Gerald V. Gibbs** (Virginia Polytechnic Institute): Quantum chemical study of bonded interactions in earth materials and related molecules

Andrey G. Kalinichev (University of Illinois): Molecular simulations of liquid and supercritical water: Thermodynamics, structure, and hydrogen bonding

James D. Kubicki (Pennsylvania State University): Calculation of vibrational properties for geoscience applications Steve Parker (University of Bath): The application of lattice dynamics and molecular dynamics techniques to minerals and their surfaces

Kevin M. Rosso (Pacific Northwest National Laboratory): Structure and reactivity of semiconducting mineral surfaces: Convergence of molecular modeling and experiment

James R. Rustad (Pacific Northwest National Laboratory): Molecular models of surface relaxation, hydroxylation, and surface charging at oxide-water interfaces

David Sherman (Bristol University): Quantum chemistry and classical simulations of metal complexes in aqueous solutions

Lars Stixrude (University of Michigan): First principles theory of mantle and core phases

John A. Tossell (University of Maryland): Calculating the NMR properties of minerals, glasses and aqueous species Yitian Xiao (ExxonMobil Research): Modeling petroleum and natural gas generation: A first principles approach

Short Course Volume: As customary for Geochemical Society and Mineralogical Society of America short courses, a short course volume will be published and will be distributed at the course. The book *Molecular Modeling Theory and Applications in the Geosciences* includes fourteen chapters authored by the speakers.

Schedule

Friday evening, May 18: Welcoming reception, 7:00 PM - 9:00 PM

Saturday May 19:

Continental breakfast, 8:00–8:30 AM Morning session, 8:30 AM – 12:00 PM Buffet lunch, 12:00–1:30 PM Afternoon session, 1:30–5:00 PM Evening open

Sunday May 20:

Continental breakfast, 8:00–8:30 AM Morning session, 8:30 AM – 12:00 PM Buffet lunch, 12:00–1:00 PM Transport to Goldschmidt Conference

| Fees | | by April 2, 2001 | after April 2, 2001 |
|------|---------------------------|------------------|---------------------|
| | Professional registration | \$150 | \$200 |
| | Student registration | \$100 | \$150 |

Practical Information

Registration fee includes GS-MSA short course session costs, welcoming reception, breakfasts, lunches, break refreshments, and *Reviews in Mineralogy and Geochemistry* volume. All short course sessions will be at the Hotel Roanoke and Conference Center. There will be an informal welcoming reception at 7:00 PM Friday evening May 18, 2001 at the same location. Complimentary bus service to the Hotel Roanoke is available from the Roanoke airport. Registration fee does NOT include room costs, other meals, or transportation costs to or from the main Goldschmidt Conference at The Homestead. Short course attendees planning on attending the Goldschmidt Conference and needing bus transportation should make bus reservations using the conference web page (http://www.lpi.usra.edu/meetings/gold2001/). These buses will be picking up short course attendees at the Hotel Roanoke after lunch on Sunday May 20. A block of discounted rooms at the Hotel Roanoke are available for both Friday and Saturday nights. Rates are \$92.00 plus taxes per night (single occupancy), \$102.00 plus taxes per night (double occupancy), plus \$10.00 per night (plus taxes) for each additional person. Attendees must make their own room reservations by calling the hotel at 540-985-5900 and asking for the Molecular Modeling Short Course room block, or by making a reservation via the hotel web site (http://www.hotelroanoke.com/). Reservations must be made by Friday April 20, 2001 in order to guarantee the discounted room rates. All short course information and registration materials can be obtained at the short course web site (http://www.sandia.gov/eesector/ GScourse.htm).

Goldschmidt Conference Session: A session entitled *Molecular Modeling in Geochemistry* will be scheduled for Monday and Tuesday May 21 and 22, 2001 as part of the Goldschmidt Conference. You are welcome to submit a contributed abstract and participate in the formal meeting.

Short Course Registration Form see next page

| Geochemical Society and Mineralogical Society of America Short |
|--|
| Course Registration Form |

Molecular Modeling Theory and Applications in the Geosciences Roanoke, Virginia, U.S.A—May 19-20, 2001

Complete and return this registration form to the Geochemical Society Business Office via e-mail, fax, regular mail, or by telephone. An electronic version of the form can be obtained through links on the short course web page (http://www.sandia.gov/eesector/GScourse.htm). Registration is limited to 120 people. Payment must accompany this form, which will be fully refunded if cancellation is received in writing by May 1, 2001.

| company this form, which whi | be fully refunded if c | ancentation is received in writing by w | lay 1, 2001. |
|--|----------------------------------|--|--------------------------|
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A new e-mail list for experimental petrologists

r. David Draper wishes to announce that an e-mail list has formed for experimental petrologists and other interested geoscientists. The list is the successor to an earlier version administered by Dr. Henry Shaw, who originated the idea in the early 1990s. Its purpose is to serve as a central point for the sharing of information on experimental materials, techniques, and results.

In addition to simple emails sent to all list members, this new version has additional features, including a calendar on which meeting information is stored, a files section where all manner of information can be housed, and sections for collections of useful links and other items.

The "owner" of the list, David Draper of NASA Johnson Space Center, Houston, Texas, can be reached for further information at david.s.draper1@jsc.nasa.gov. The URL for the group is http://groups.yahoo.com/group/ExPet. Users following that link who do not yet have an account with Yahoo register for a free account, and membership in the list is granted automatically. Draper does not moderate or filter posts to the group in any way, and all group features are accessible to all group members. Yahoo has a robust privacy policy, and so far there have been no reports of anyone's email address falling into the hands of spammers. All geoscientists with an interest in experimental work are encouraged to join the list.

Workshop on Solid Solutions in Silicate and Oxide Systems of Geological Importance

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Welcome New Members

he following individuals joined (or rejoined after a long hiatus) MSA during January 2, 2001 through January 28, 2001. We welcome them to the Society. The areas of interest are: Mineralogy (MI), Crystallography/Crystal Chemistry (CC), Material Properties (PP), Igneous Petrology (IP), Metamorphic Petrology (MP), Sedimentary Petrology (SP), Geochemistry (GE), Phase Equilibria (PE), Economic Geology (EG), Clay Mineralogy (CM), Industrial Mineralogy (IM), Environmental Mineralogy (EM), Gems (GM), Planetary Materials (PM), Teaching (TC), Topologic or Descriptive Mineralogy (TP), **Biological-Mineral Interactions** (BM), and others as indicated.

If you know of someone who would like or should join MSA, give them the membership application that appears in this issue of *The Lattice*, or is available from either MSA's web site (http://www. minsocam.org) or the MSA Business Office, 1015 Eighteenth St NW Ste 601, Washington, DC 20036-5212, USA.

rediningsih, Miss Yulini, KAVLING TNI-AL, Jalan Teluk Palu Blok A/3 No. 16, Pondok Bambu, Jakarta 13430, INDO-NESIA. Ph: +62 (21) 8620393. E-mail: y.arediningsih @auckland.ac.nz (S-01). MI, IP, GE, EG, IM,

Baker, Prof. Leslie L., Rocky Mountain Col lege, Dept Earth & Environmental Sci, 1511 Poly Dr, Billings MT 59102-1796. Ph: (406) 657-1101. Fax: (406) 259-9751. E-mail: leslie baker@ sigmaxi.org (M-01). IP, GE, PE, EM, PM, TC,

Bennett , Mr. Ryan T., 818 Partridge Cir, Golden, CO 80403-1544. Ph: (303) 384-3392. E-mail: rtb @rmi.net. (11-01). IP, EG, IM.

Boffa Ballaran, Dr. Tiziana, Univ Bayreuth, Bayerisches Geoinstitut, Bayreuth D-95440, GERMANY. Ph: +49 (921) 553738. Fax: +49 (921) 553769. E-mail: tiziana.boffa-ballaran@ uni-bayreuth.de (M-01). MI, CC, PP, PE,

Byrne, Mr. Patrick J., 2431 Lancashire Dr Apt 2A, Ann Arbor MI 48105-1361. Ph: (734) 623-6310. E-mail: pjbyrne@engin.umich. edu (S-01). MI, EM, OTHER, NUCLEAR TOPICS

ampbell, Mr. Brian J., 608 E Lindsey St Apt B, Norman OK 73069-4776. Ph: (405) 325-9489. Email: applecore@ou.edu (S-01). MI, GE, EM, GM, PM, BM,

Carter, Mr. Jerry K., 38 Day St Apt 42, Somerville MA 02144-2855. Ph: (617) 428-4444. Fax: (617) 428-1122. Email: heliodor@ earthlink.net (M-01). MI, GM, PM, BM,

Catalina, Ms. Maria, 821 Koshland Way, Santa Cruz CA 95064-1008. Ph: (831) 458-0405. Fax: (831) 459-3704. E-mail: m_cat@cats. ucsc.edu (S-01). MI, CC, PP, SP, CM, EM, PM, TC, BM,

Cusimano, Ms. Maryann, 8558 Smith Ln, College Station TX 77845-7548. Ph: (409) 862-2469. E-mail: mac4879@geo. tamu. edu (S-01). MI, GE, CM, EM, GM,

avis, Mr. Kevin James, Virginia Tech, 4044 Derring Hall, Blacksburg VA 24061-0000. Ph: (540) 231-8074. Fax: (540) 231-3386. Email: kdavis2@vt.edu (S-01). GE, MI, CC, PP, BM,

De Azevedo, Mr. Antonio C., Purdue University, Agronomy Department, 1150 Lilly Hall, West Lafayette IN 47907-0000. Ph: (765) 494-4773. Fax: (765) 496-2926. E-mail: aazevedo@purdue.edu (S-01). MI, CC, GE, PE, CM, EM, TC, BM, OTHER, S OIL MINER-ALOGY

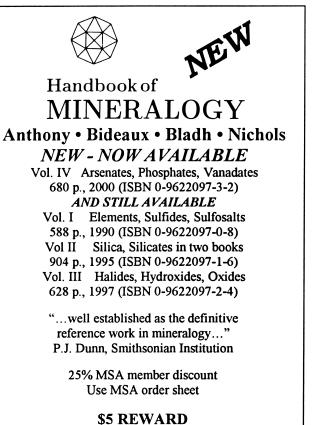
De Capitani, Dr/Prof Christian E., Universitat Basel, Mineralogisch-Petrographisches Inst, Bernoullistrasse 30, Basel CH-4056, SWITZERLAND. Ph: +41 (61) 267 3621. Fax: +41 (61) 267 2881. E-mail: christian. decapitani@unibas.ch (M-01). MI, CC, PP, MP, GE, PE, IM, EM, TC,

Transform arrell, Mr. Shannon P., Univ of Western Ontario, Dept of Earth Sciences, London, ON N6A 5B7, CANADA. Ph: (519) 661-3187. Fax: (519) 661-3198. E-mail: spfarrel@julian.uwo.ca. (S-01) MI, CC, PP, PE, IM, GM, PM, TC, MS

Fuller, Mr. Roy W., 9315 Northgate Blvd Apt 209, Austin TX 78758-6175. Ph: (512) 832-6975. E-mail: rwf6@ mail. utexas.edu (S-01). MI, CC, PP, IP, MP, GE, PE, CM, EM, PM, TP, BM, Funakoshi, Dr. Ken-ichi, Japan Synchrotron Radiation Inst, Koto 1-1-1, Mikazuki, Sayo-gun, Hyogo 679-5198, JA-PAN. Ph: +81 (791) 58 2632. Fax: +81 (791) 58 2740. E-mail: funakosi@spring8. orjp (M-01). MI, PP,

Furgal, Ms. Stephanie A., New Mexico State Univ, Dept of Geological Sciences, Box 3AB, Las Cruces NM 88003-0000. Ph: (505) 646-2708. Fax: (505) 646-1056. E-mail: sfurgal@nmsu.edu (S-01). MI, IP, MP, EM,

Lasmacher, Dr. Ulrich A., Max-Planck-Inst Fur Kernphysik, Forschungsstaelle Archaeo-metrie, P.O. Box 103980, Heidelberg D-69029, GERMANY. Ph: +49



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Gomes, Prof. Maria Elisa, Univ de Tras-os-Montes e Alto Douro, Dep. de Geologia, Vila Real, 5001-911, PORTUGAL. . Ph: +351 259350261. Fax: +351 259350480. E-mail: mgomes @utad.pt. (M-01) CC, PP, IP, MP, SP, GE, PE, CM, EM, GM, TP, MS

Gray, Mr. Walter M., Univ of North Carolina, Dept of Geological Sci, CB #3315, Chapel Hill NC 27599-3315. Ph: (919) 933-5739. E-mail: wgray@ email.unc.edu (S-01). MI, CC, IP, MP, GM, TC,

Hartmann, Dr. Thomas, Los Alamos Nat'l Lab, Carlsbad Operations, 115 N Main St, Carlsbad NM 88220-0000. Ph: (505) 628-3934. Fax: (505) 628-3238. E-mail: hartmann@lanl. gov (M-01). MI, CC, PP, GE, CM, EM, TC, TP, BM,

Hauzenberger, Dr. Christoph A., Universitaet Mainz, Inst fuer Geowissen-schaften, Becherweg 21, Mainz D-55099, GERMANY. Ph: . Fax: +49 (6131) 392 3070. Email: hauzenbe@mail.uni-mainz. de (M-01). MI, CC, PP, IP, MP, SP, GE, PE, EG, CM, IM, EM, GM, PM, TC, TP, BM, EXPERIMEN-TAL PETROLOGY

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Huff, Dr. Warren D., Univ of Cincinnati, Dept of Geology, Cincinnati OH 45221-0013. Ph: (513) 556-3731. Fax: (513) 556-6931. E-mail: warren.huff@uc.edu (M-01). MI, IP, GE, CM, TC,

ugo, Ms. Pedro J., Univ of Alberta, Dept Earth & At mospheric Sci, Edmonton AB T6G 2E3, CANADA. Ph: . Fax: (780) 492-2030. E-mail: pjugo@ualberta.ca (S-01). MI, CC, IP, GE, PE, EG, TC,

avner, Dr. Abby, Lamont Doherty Earth Observatory, 61 Route 9W, Palisades NY 10964-1707. Ph: (845) 365-8907. Fax: (845) 365-8155. E-mail: kavner@ Ideo.columbia.edu (M-01). MI, PP, IP, GE, PE, GM, PM, BM,

Kaylor, Mr. Ahren M., 308 S Drake Rd Apt C3, Kalamazoo MI 49009-1138. Ph: (616) 388-4648. E-mail: s8kaylor@umich. edu (S-01). EG, EM, GM, PM, TC, TP, BM, OTHER, EARTH SCIENCES

Krekeler, Mr. Mark P., Univ of Illinois, Dpet Earth & Envn Sci, M/C 186, Chicago IL 60607-7059. Ph: (312) 996-3154. Email: rhodochrosite@email. msn.com (S-01). MI, CC, PP, SP, CM, IM, EM, TC, BM,

ake, Dr. Charles H., In diana Univ of Pennsylva nia, Dept of Chemistry, Indiana, PA 15705-0000, Ph: ((724) 357-2398. E-mail: lake@ grove.iup.edu. (M-01) CC

Lane, Mr. Edward D., 1100 E 32nd St Apt 201, Austin TX 78722-2250. Ph: (512) 653-7821. E-mail: edlane@ mail.utexas.edu (S-01). MI, CC, PP, IP, MP, GE, PE, TC, MS,

Lee, Ms. Aletha J., 911 22nd Ave S Apt 163, Minneapolis MN 55404-2238. E-mail: leex1254@ tc.umn. edu (S-01). MI, MP, EM, TC,

Lewis, Mr. Jared F., 7315 Brompton St Apt 223B, Houston TX 77025-2144. Ph: (713) 348-3272. E-mail: jflewis@ rice.edu (S-01). IP, GE, TC,

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Liu, Mr. Yun, 431 Chapin Complex, Stony Brook NY 11790-3364. Ph: (631) 216-2066. Fax: (631) 632-8240. E-mail: yunliu@ic.sunysb.edu (S-01). MI, CC, PP, IP, MP, GE, PE, CM, IM, EM,

Lopez, Ms. Yvette C., New Mexico State Univ, Dept of Geological Sciences, Box 3AB, Las Cruces NM 88003-0000. Ph: (505) 646-2708. Fax: (505) 646-1056. E-mail: yvelopez@ nmsu.edu (S-01). MI, IP, EM, ader, Dr/Prof Werner, Univ of Bonn, Inst Fur Anor ganische Chemie, Roe merstrasse 164, Bonn D-53117, GER-MANY. Ph: +49 (228) 734203. Fax: +49 (228) 734205. E-mail: mader@uni-bonn.de (M-01). CC, MP,

Mattielli, Dr. Nadine, Univ Libre de Bruxelles-DSTE, 50 Av F.D. Roosevelt, CP 160/02, Brussels B-1050, BELGIUM. Ph: +32 (2) 650-2269. Fax: +32 (2) 650-2226. E-mail: nmattiel@ ulb. ac.be (M-01). IP, GE, TC,

Mattinson, Mr. Christopher G., Stanford Univ, Dept of Geology, Stanford CA 94305-2115. Ph: (650) 736-2215. E-mail: cgm@pangea. stanford.edu (S-01). MI, CC, IP, MP, GE, PE,

McCammon, Mr. Raymond W., 20619 Martha St, Woodland Hills, CA 91367-6727, Ph: (512) 477-5566. Email: kn6tfx@ aol.com. (M-01) MI, CC, GM.

McCollam, Ms. Bridget E., New Mexico State Univ, Dept of Geological Sciences, Box 3AB, Las Cruces NM 88003-0000. Ph: (505) 646-2708. Fax: (505) 646-1056. E-mail: brmccoll@nmsu. edu (S-01). MI, CC,

McCall-Elledge, Ms. Patti Jo, 3155 Scenic Lake Dr Apt 20, Ann Arbor MI 48108-4213. Ph: (734) 973-6736. E-mail: pjmccall@umich.edu (S-01). MI, GE, EM, PM,

Meth, Ms. Charna E., 302 E 34th St Apt 204, Austin TX 78705-1647. Ph: (512) 494-8487. E-mail: charna@ mail.utexas.edu (S-01). MI, MP,

Moloy, Mr. Eric C., 4735 Cowell Blvd Apt 94, Davis CA 95616-4475. Ph: (530) 219-1765. E-mail: ecmoloy @ucdavis.edu (S-01). CC, PP, CM, IM, OTHER, ZEOLITES

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Svihla, Ms. Vanessa L., 2919 West Ave Apt 408, Austin TX 78705-3529. Ph: (512) 293-8278. E-mail: vsvihla@ hotmail.com (S-01). MP, TC, OTHER, STRUCTURAL GEOLOGY

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Tomkins, Mr. Andrew G., Australian Nat'l Univ, Geology Department, Canberra ACT 200, AUSTRALIA. Ph: +61 (2) 6125 4303. Fax: +61 (2) 6125 5544. E-mail: andy@geology.-anu.edu. au (S-01). MP, GE, PE, EG, PM,

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Veksler, Dr. Ilya V., GeoForschungsZentrum Potsdam, Telegrafenberg B-120, Potsdam D-14473, GERMANY. Ph: +49 (331) 288 1425. Fax: +49 (331) 228 1474. E-mail: veksler @gfz-potsdam.de (M-01). MI, IP, GE, PE,

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Winkle, Ms. Amy L., 913

President's Letter, Continued from page 2

changes in most North American universities. Originally the undergraduate course sequence may have included mineralogy (as a first requirement in the major), optical mineralogy (as a prerequisite to subsequent petrology/petrography courses), igneous and metamorphic petrology, sedimentary petrology, and elective offerings in X-ray diffraction techniques, and advanced mineralogy (generally at the senior level). Since then, many departments have reduced the mineralogy core sequence to a onesemester course in mineralogy, with a required laboratory. If such a single course (including the laboratory) comes with an increased number of credits, such as 5 or 6 credits, much of what is basic to mineralogy can still be taught. However, if the total number of credits has been reduced (in the single mineralogy offering) to something like 3 credits (including a laboratory), or if the subject matter emphasizes mainly "minerals and rocks" (with laboratories that stress only hand specimen identification) much of what are considered basic concepts in mineralogy, crystal chemistry, and crystallography cannot be covered.

These changes were brought about, I believe, because some of our colleagues simply think that the subject of mineralogy is outdated or irrelevant, and because of a common desire to accommodate new course offerings. But because the required number of courses (in a core curriculum) is generally fairly fixed, and cannot be expanded (within a four-year degree program) subject matter that was originally part of the core was eliminated or deemphasized. Almost everywhere, the well-established course sequence in mineralogical and petrological subjects was severely reduced in order to make room for new offerings.

This then raises the broader question of "what should be taught" in a basic, one-semester mineralogy course. This might be addressed by asking the question of "what should a geology (or environmental science) B.A. or B.S. recipient be prepared to deal with?," be it in subsequent graduate school, or as a professional in the work force. My own, short answer to this, is that any student who has taken a single undergraduate mineralogy course, should be reasonably comfortable in dealing with most of what appears in Reviews in Mineralogy (published by the Mineralogical Society of America) and such reference volumes as those written by W.A. Deer, R.A. Howie, and J. Zussman (the various volumes that are part of Rock-forming Minerals). To be reasonably comfortable in consulting any of these volumes, the new graduate must have had considerable grounding in crystal chemistry, crystal structure, mineral behavior, and crystallography, and he or she must have some fundamental understanding of mineral stability and/or mineral assemblage diagrams. As part of this background, I think, a new graduate should have some familiarity with space groups and their notation, which is interwoven into all mineral descriptions in every one of the references mentioned above.

Monaca Rd, Monaca PA 15061-

2918. Ph: (724) 378-3878. E-

mail: satinspar@ hotmail.com

246-6076. E-mail: tony.yu@

sunysb. edu (S-01). MI, CC, PP, PE,

IM, EM, GM, PM, TC, TP,

7u, Mr. Tony, 1341 Stony

Brook Rd, Stony Brook

NY11790-2201. Ph: (631)

(S-01). MI, CC, MP, PE, BM,

The reduction in mineralogical subject matter in the undergraduate curriculum has come about even though mineralogy is extremely closely tied, and is indeed a necessary prerequisite, to subsequent courses in petrology, economic geology, geochemistry, and environmental mineralogy. As Frank Hawthorne stated so clearly in his 1993 paper entitled "Minerals, mineralogy, and mineralogists: past, present, and future "(The Canadian Mineralogist, v. 31, p. 253-296) Minerals are the basic stuff of the Earth, and their study will always remain at the core of the Earth Sciences. Anyone who teaches mineralogy in a geology department will agree with this statement, but nonetheless mineralogy has a much smaller presence (or visibility) in the core curriculum than it had twenty years ago.

There is yet another factor that affects the quality of teaching of mineralogy. Fewer and fewer mineralogists (and/or crystallographers) are being trained at the Ph.D. level. Further-

MSA distinguished lecturers for 2001-2002

Since its inception the Lecture Program of the Mineralogical Society of America has proven to be a great success. The varied and interesting lectures presented by MSA Distinguished Lecturers have been appreciated by students and faculty at many colleges and universities in the United States and Canada. The Council of the Mineralogical Society is again offering the program for the 2001-2002 academic year with the arrangement that the MSA will pay travel expenses of the Lecturers, and the host institutions will be responsible for local expenses, including accommodation and meals. For the second time this year MSA has expanded the program to include 3 lecturers, one of whom resides in Europe, and is encouraging European universities to request lecturers. Depending on the response, one or more lecture tours will be arranged in Europe. The Mineralogical Society of America is pleased to announce that its Distinguished Lecturers for 2001-2002 are:

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Continued from page 16

more, departmental advertisements for a new hire in Geology may read: "Ph.D. in hydrology required. Candidate will be required to develop a vigorous research program in this field of expertise. The candidate will also be responsible for the undergraduate mineralogy course." The reduction in training and research in mineralogy and/or crystallography at the Ph.D. level, and the assignment of instructors who have quite different research interests from that which relates to mineralogy, generally means that the subject of mineralogy is probably not taught at the level and to the depth that it should be.

All of the above trends have affected the undergraduate mineralogy course as it is now offered. Mineralogy can be a very stimulating and exciting field to undergraduates if it is well taught. It can open venues to materials science if the subject matter is taught with integrity. I trust that we all agree that a 3credit course on "Rocks and Minerals," or "Earth Materials" (with the main emphasis on descriptive aspects of the subject, as well as hand specimen identification) is not the correct preparation for graduate school or employment after graduation. If the lectures in the undergraduate mineralogy course are not centered on concepts in crystal chemistry, crystal structure, crystallography, and paragenesis, I conclude that we are not doing our undergraduates any favors.

What must we conclude from all this? Even though we as mineralogical professionals may be able to convince our students of the significance and relevance of mineralogy to the overall field of earth science, it appears that we have been remiss in not convincing our departmental colleagues of the central and highly significant role of mineralogy to the curriculum. Examples of the immediate applicability of mineralogic/crystallographic and crystal chemical concepts to topics of great current interest and excitement are biomineralogy, behavior of mineral surfaces, nanoscale processes, and mineral-fluid interactions. Clearly, we must do a much better job, in the future, of convincing our colleagues of the need for maintaining a rigorous mineralogic curriculum at the undergraduate level.

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Meeting Calendar 2001

April

8–12 Symposium on "Transformation Processes in Minerals" at the European Union of Geosciences meeting. Strasbourg, France. Details: WWW: http://eost.ustrasbg.fr/EUG

May

20–24 11th Annual V. M. Goldschmidt Conference. Roanoke, VA. Details: Bob Bodnar (bubbles@vt.edu) or Mike Hochella (hochella@vt.edu).

27–30 St. John's 2001, Geological Association of Canada–Mineralogical Association of Canada Annual Joint Meeting. St. John's, New Foundland, Canada. Details: St. John's 2001, c/o Department of Mines and Energy, St. John's, New Foundland, A1B 4J6; Tel. 709-729-2301; Fax: 709-729-3493; E-mail: dmp@zeppo. geosurv.gov.nf.ca.

June

9–24 Field Course on Rare Earth Pegmatites. Madagascar. Details: Federico Pezzotta - Museo Civico di Storia Naturale, Corso Venezia 55, 20121 Milan, Italy. E-mail: fpezzotta@yahoo.com, FAX: (++39) 02 76022287, Phone: (++39) 02 781312 Wm. B. "Skip" Simmons – University of New Orleans, Department of Geology & Geophysics, New Orleans, LA 70148, USA. E-mail: wsimmons@uno.edu, FAX: (504) 280 7396, Phone: (504) 280 6791

24–28 Earth Systems Processes–A Global Meeting. Edinburgh, Scotland. Details: Ian Dalziel, E-mail: Ian@utig.ig.utexas.edu or Ian Fairchild, E-mail: i.j.fairchild@keele.ac.uk, WWW: http://www.geolsoc. org.uk.

24–29 Workshop on Solid Solutions. Lubeck, Germany. Details: Charles Geiger. E-mail: chg@min.unikiel.de, WWW: www.ifg.uni-kiel.de/Veranstaltungen/ mader.html.

July

1–6 Advances in Environmental Materials. Singapore. Details: Tim White, Environmental Technology Institute, Innovation Centre, NTU, Block 2, Unit 237, Nanyang Drive, Singapore 637723. E-mail: tjwhite@eti.org.sg, FAX: 65-792 1291, Phone: 65-794 1509; WWW: http://www.mrs.org.sg/icmat2001.

August

26–29 6th **Biennial SGA meeting.** Krakow, Poland. Details: Wojciech Mayer, University of Mining and Met-

allurgy, Faculty of Geology, Geophysics and Environmental Protection, av. Mickiewicza 30, 30-059 Krakow, Poland. Tel.: 48-12-6172385, Fax: 48-12-63332936, E-mail: wmayer@geol.agl.edu.pl, WWW: http:// galaxy.uci.agh.edu.pl/~sga.

September

1-7 Sixth International Eclogite Conference in Japan. Niihama, Ehime, Japan. Details: Masaki Enami, Department of Earth and Planetary Sciences, Graduate School of Science, Nagoya University, Nagoya 464-8602, Japan; Tel. and fax 81-52-789-3005 E-mail: enami@eps.nagoya-u.ac.jp; WWW: ganko.eps.nagoya-u.ac.jp/iec2001/index.html.

6–8 CL 2001 – Cathodoluminescence in Geosciences: New Insights from CL in combination with other techniques. Freiberg, Germany. Details: CL 2001 Secretariat, Freiberg University of Mining and Technology, Department of Mineralogy, Brennhaus-gasse 14, D-09596 Frei-berg, Germany; Tel.: +49-(0)3731-392628, Fax: +49-(0)3731-393129 E-mail: goetze@ mineral. tu-freiberg.de; WWW: www. mineral.tu-freiberg. de □

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Deadline

Material for the May 2001 Lattice is April 13, 2001.

Contributions may be sent to Andrea Koziol via surface mail at the Department of Geology, University of Dayton, Dayton, OH 45469-2364 or via e-mail at koziol@ notes.udayton.edu.

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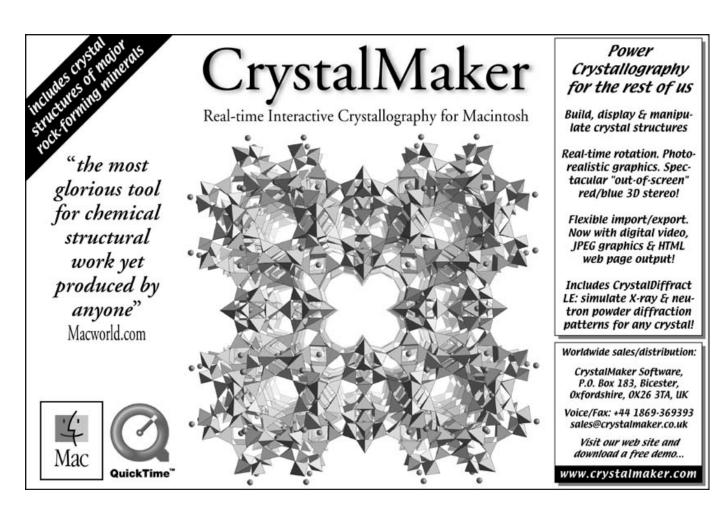
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